

Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

PMRA Document Number 1686946
PMRA Submission Number 2008-0431

EPA MRID Number 47611201

Data Requirement: PMRA Data Code: 8.2.3.4.4
EPA DP Barcode: 360246
OECD Data Point: IIA 7.1.2, IIA 7.2.4
EPA Guideline: 835.4200

Test material:

Common name: Saflufenacil.

Chemical name:

IUPAC name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.


CAS name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS No: 372137-35-4.


Synonyms: BAS 800 H, BAS800H, BAS 800H, CL No. 433379, 4054449, AC 433,379.

SMILES string: N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(Cl)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

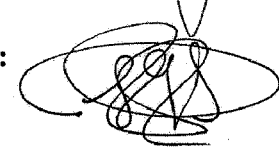
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Company Code: BAZ

Active Code: SFF

Use Site Category: 13 and 14

EPA PC Code: 118203

CITATION: Panek, M. and A. Pyles. 2008. Anaerobic soil metabolism of ¹⁴C-BAS 800 H. Unpublished study performed, sponsored and submitted by BASF Corporation, Research Triangle Park, North Carolina (p. 1). BASF Study No.: 332554. Registration Document No.: 2008/7015021. Experimental start date June 30, 2008, and completion date November 20, 2008 (p. 12). Final report issued December 15, 2008 (p. 1).



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Active Code:

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EPA PC Code: 118203

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EXECUTIVE SUMMARY

The biotransformation of [phenyl- ^{14}C]- and [uracil-4- ^{14}C]-labeled N' -{2-chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}- N -isopropyl- N -methylsulfamide (saflufenacil, BAS 800 H; radiochemical purities $\geq 95\%$ and $\geq 98\%$, respectively) was studied in a loamy sand soil (pH 6.0, organic carbon 0.9%) from Wisconsin for 75 days under anaerobic conditions (flooding, nitrogen atmosphere) in darkness at $25 \pm 1^\circ\text{C}$ following 17 days of aerobic incubation. Soil moisture content at study initiation was adjusted to 99% of field capacity at 1/3 bar. [^{14}C]Saflufenacil was applied at a nominal rate of 1.07-1.12 mg a.i./kg (equivalent to *ca.* 1.20 kg a.i./ha). The study was conducted in accordance with USEPA Pesticide Assessment Guidelines, Subdivision N §162-2 and in compliance with USEPA FIFRA GLP standards (40 CFR Part 160). The test apparatus consisted of Nalgene polypropylene containers (not further described) connected to a continuous flow-through (CO_2 -free air, flow rate not reported) system with traps for the collection of CO_2 (0.5N NaOH) during the aerobic phase of the incubation. During the anaerobic phase, the treated systems were connected to a continuous flow-through (humidified nitrogen, flow rate not reported) system with traps for the collection of CO_2 (0.5N NaOH) and volatile organics (ethylene glycol), except at 6-14 days post-flooding when the systems were maintained sealed under static conditions. Following treatment, duplicate incubation vessels of treated soil were taken for analysis after 0, 14 and 17 days of aerobic incubation, then after conversion to anaerobic conditions, single or duplicate water-soil systems were taken at 23, 28, 35, 43, 51, 59, 77 and 92 days posttreatment (6, 11, 18, 34, 42, 60 and 75 days post-flooding, respectively). Water layers, when present, were centrifuged, decanted and analyzed directly. Soil was extracted once with acetonitrile, followed by twice with acetonitrile:water (70:30, v:v). Extracts were combined and concentrated *in vacuo* and via N -Evap for chromatographic analysis. Water layers, extracts, extracted soil and volatile trapping solutions were analyzed for total radioactivity using LSC. Water layer and soil extract samples were analyzed by reverse-phase HPLC. Seven reference standards, in addition to parent saflufenacil, were available for identification purposes (see Table 5 below). Identifications of isolated parent saflufenacil and major transformation products were confirmed via LC/MS and LC/MS/MS.

The test conditions presented in the study appear to have been maintained throughout the 92-day incubation, with the exception that air-flow (aerobic phase) to the phenyl-label treated Replicate 2 sample series (sample "train") was greater than to the Replicate 1 sample series due to a malfunctioning manifold. The study authors believed that moisture levels of the Replicate 2 treated soil samples in the vessels closest to the air entry were impacted to the point that soil metabolic activity was significantly decreased in the Replicate 2 systems collected at 35-92 days posttreatment (18-75 days post-flooding). For the purposes of this DER, the results of phenyl-label treated Replicate 2 systems were considered invalid and were not reported or included in calculations.

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Conditions in the soil layers (both labels) were reducing to moderately reducing with a mean redox potential of -34 ± 88 mV. Dissolved oxygen at the water-soil interface averaged 0.16 ± 0.04 mg/L, while water layer pH levels averaged 5.3 ± 0.3 .

Labels combined. Overall recovery of radiolabeled material averaged $98.5 \pm 2.2\%$ (range 92.6-105.6%) of the applied, with no pattern of decline in recoveries for either label throughout the study. After flooding at 17 days posttreatment, [^{14}C]residues readily partitioned from the soil to the water layer with distribution ratios (water:soil, mean, $n = 4$ or 2) of 2:1 at 6 days post-flood (23 days posttreatment), then remained at 3:1 thereafter. Flooding significantly slowed the overall rate of degradation with saflufenacil in the soil decreasing from a mean 106.6% of the applied at day 0 posttreatment to 42.6% at 17 days, just prior to flooding, then post-flooding was 37.5% in the total system at 23 days posttreatment (6 days post-flood) and 33.5% at 92 days (75 days post-flood). In the water layer, saflufenacil gradually increased from 26.3% at 23 days (6 days post-flood) to 39.1% at 43 days (26 days post-flood) and was 26.2% at 92 days (75 days post-flood). In the soil post-flooding, saflufenacil was 11.2% at 23 days (6 days post-flood) and 7.3% at 92 days (75 days post-flood). Under anaerobic conditions, reviewer-**observed DT50** values for saflufenacil were <6 days post-flooding in the soil and >75 days post-flooding in the water layer and total system, with reviewer-observed DT90 values of >75 days post-flooding in the water, soil and total system. In the soil, reviewer-calculated **linear** and **nonlinear SFO DT50s** were 47 days ($r^2 = 0.38$) and 11 days ($r^2 = 0.81$), respectively. In the total system, reviewer-calculated non-linear SFO DT50/DT90 values were 217/ 721 days. Reviewer-calculated half-lives were not determined for saflufenacil in the water layers due to insufficient dissipation post-flooding.

Three major nonvolatile transformation products,

- N'-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-tetrahydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide (M800H08),
- N'-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropylsulfamide (M800H01), and
- N'-[2-chloro-4-fluoro-5-(2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)-4-fluorobenzoyl]-N-isopropyl-N-methylsulfamide (M800H02), and

four minor products,

- N-{4-chloro-2-fluoro-5-[(isopropyl(methyl)amino)sulfonyl]amino}carbonyl]phenyl}-4,4,4-trifluoro-3,3-dihydroxybutanamide (M800H15-ketohydrate) and
- 3-[(4-chloro-2-fluoro-5-[(isopropyl(methyl)amino)sulfonyl]amino)carbonyl]aniline}-carbonyl(methyl)amino]-4,4,4-trifluorobutanoic acid (M800H22),
- N-{4-chloro-2-fluoro-5-[(isopropyl(methyl)amino)sulfonyl]amino}carbonyl]phenyl}-N'-methylurea (M800H07), and
- trifluoroacetic acid,

were detected. M800H08, M800H01, M800H02, M800H15-ketohydrate and M800H22 were detected with both labels, M800H07 was detected in phenyl-label treated systems and trifluoroacetic acid in uracil-label treated systems. **M800H08** was a mean 16.7% of the applied in the soil at 17 days posttreatment, then post-flooding was a maximum mean 21.1% in the total

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system (16.5% water, 4.6% soil) at study termination. **M800H01** was a mean 10.1% in the soil at 17 days, then post-flooding was a maximum mean 13.3% in the total system (6.7% in both water and soil) at 43 days (26 days post-flood) and was 9.8% (8.1% water, 1.8% soil) at study termination. **M800H02** was a mean 11.6% of the applied in the soil at 17 days, then post-flooding was a maximum mean 18.0% in the total system (14.8% water, 3.2% soil) at study termination. Under anaerobic conditions (post-flooding) in the total system, **M800H15-ketohydrate** was detected at a maximum ($n = 1$) 1.9% (maximum 1.6% in water, 1.2% soil), **M800H22** at 1.6% (1.6% water, 0.4% soil), **M800H07** at 4.4% (3.3% water, 1.3% soil), and **trifluoroacetic acid** at 4.0% (3.4% water, 1.0% soil). Total unidentified [^{14}C]residues, comprised of several components, were detected at maximums (both labels) of 7.5-10.1%, 4.3-7.5% and 9.5-12.2% in the water layer, soil and total system, respectively, with no individual component detected at >4.5%, 4.3% and 4.9%, respectively. Extractable [^{14}C]residues decreased from a mean 99.8% of the applied at day 0 to 91.2% at 17 days, then post-flooding were 26.0% at 23 days (6 days post-flood) and 20.0% at study termination. Nonextractable [^{14}C]residues were a mean 0.4% of the applied at day 0 and 3.9-6.1% thereafter. $^{14}\text{CO}_2$ and [^{14}C]volatile organics were minimal totaling $\leq 0.5\%$ and $\leq 0.3\%$ of the applied, respectively, at study termination.

[Phenyl- ^{14}C]saflufenacil treated system. [^{14}C]Saflufenacil in the soil decreased from an average of 99.1% of the applied at day 0 posttreatment to 41.0% at 17 days, just prior to flooding, then in the total system post-flooding was 31.6% at 23 days posttreatment (6 days post-flood) and 32.0% at 92 days (75 days post-flood). In the water and soil post-flooding, [^{14}C]saflufenacil averaged 21.5% and 10.1% of the applied, respectively, at 23 days posttreatment (6 days post-flood) and 25.7% and 6.3%, respectively, at 92 days (75 days post-flood).

M800H08 was 15.8-20.2% of the applied in the soil at 14-17 days posttreatment, then post-flooding was 14.6% in the total system (10.1% water layer, 4.5% soil) at 23 days (6 days post-flood), 14.1-25.1% (10.3-18.7% water layer, 3.8-7.5% soil) at 28-35 days (11-18 days post-flood) and 17.5-25.4% (14.1-20.0% water layer, 3.4-5.4% soil) at 92 days (75 days post-flood). **M800H01** was 7.5-14.1% in the soil at 14-17 days posttreatment, then post-flooding was 12.6% in the total system (9.4% water layer, 3.2% soil) at 23 days (6 days post-flood) and 7.1-10.0% (5.8-8.2% water layer, 1.3-1.8% soil) at 92 days (75 days post-flood). **M800H02** was 5.4-18.0% in the soil at 14-17 days posttreatment, then post-flooding was 16.4% in the total system (12.8% water layer, 3.6% soil) at 23 days (6 days post-flood) and 9.6-24.0% (8.3-19.8% water layer, 1.3-4.2% soil) at 92 days (75 days post-flood). **M800H07** was a maximum 3.7% in the soil at 17 days, then post-flooding was maximums of 3.3%, 1.3% and 4.4% in the water, soil and total system, respectively. **M800H15-ketohydrate** was a maximum 2.3% in the soil at 14 days, then post-flooding was maximums of 1.1%, 0.5% and 1.5% in the water layer, soil and total system, respectively. **M800H22** was detected only in the soil post-flooding at $\leq 0.4\%$. Total unidentified [^{14}C]residues, comprised of several components, were detected at maximums of 7.5% in the water layer and soil and 9.5% in the total system, with no individual component detected at >3.9%, 4.0% or 4.9% in the water layer, soil or total system, respectively.

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Extractable soil [^{14}C]residues were 99.5% (n = 2) of the applied at day 0 and 88.7-93.8% at 14-17 days, then post-flooding gradually decreased from 26.8% at 23 days (6 days post-flood) to 19.8-20.0% at 92 days (75 days post-flood). Nonextractable soil [^{14}C]residues were 0.5% (n = 2) of the applied at day 0 and 3.5-7.5% at 14-92 days. At study termination (92 days), volatilized $^{14}\text{CO}_2$ and volatile [^{14}C]organic compounds totaled 0.1% of the applied and were not detected, respectively.

[Uracil-4- ^{14}C]saflufenacil treated system. [^{14}C]Saflufenacil in the soil decreased from an average of 114.3% of the applied at day 0 posttreatment to 44.3% at 17 days, just prior to flooding, then in the total system post-flooding was 43.4% at 23 days posttreatment (6 days post-flood) and 35.1% at 92 days (75 days post-flood). In the water and soil post-flooding, [^{14}C]saflufenacil averaged 31.1% and 12.3% of the applied, respectively, at 23 days posttreatment (6 days post-flood) slowly decreasing to 26.8% and 8.3%, respectively, at 92 days (75 days post-flood). M800H08 was 11.8-17.4% of the applied in the soil at 14-17 days posttreatment, then post-flooding was 14.5% in the total system (10.1% water layer, 4.4% soil) at 23 days (6 days post-flood), 12.7-22.6% (8.5-18.0% water layer, 3.3-5.8% soil) at 28-59 days (11-42 days post-flood), 21.0-23.9% (15.3-18.5% water layer, 5.4-5.7% soil) at 77 days (60 days post-flood) and 17.9-23.5% (13.5-18.5% water layer, 4.4-5.0% soil) at 92 days (75 days post-flood). M800H01 was 9.0-12.3% in the soil at 14-17 days posttreatment, then post-flooding was 9.7% in the total system (7.4% water layer, 2.3% soil) at 23 days (6 days post-flood) and 9.9-12.2% (7.9-10.3% water layer, 1.9-2.0% soil) at 92 days (75 days post-flood). M800H02 was 8.4-14.4% in the soil at 14-17 days posttreatment, then post-flooding was 15.8% in the total system (13.0% water layer, 2.8% soil) at 23 days (6 days post-flood), 12.6-22.5% (9.8-18.5% water layer, 2.8-4.6% soil) at 28-77 days (11-60 days post-flood) and 17.0-21.3% (13.9-17.0% water layer, 3.1-4.3% soil) at 92 days (75 days post-flood). M800H15-ketohydrate was a maximum 1.7% in the soil at 14 days, then post-flooding was maximums of 1.6%, 1.2% and 1.9% in the water layer, soil and total system, respectively. M800H22 was detected only post-flooding at maximums of 1.6% in the water and total system and 0.2% in the soil. Trifluoroacetic acid was a maximum 6.9% in the soil at 17 days, then post-flooding was maximums of 3.4%, 1.0% and 4.0% in the water layer, soil and total system, respectively. Total unidentified [^{14}C]residues, comprised of several components, were detected at maximums of 10.1%, 4.3% and 12.2% in the water layer, soil and total system, respectively, with no individual component detected at >4.5% in the water layer and total system, or >4.3% in the soil.

Extractable soil [^{14}C]residues were 99.7-100.4% of the applied at day 0 and 91.4-94.7% at 14-17 days, then post-flooding were 25.1% at 23 days (6 days post-flood) and 19.5-20.6% at 92 days (75 days post-flood). Nonextractable soil [^{14}C]residues were 0.3% (n = 2) of the applied at day 0 and 3.3-5.7% at 14-92 days. At study termination, volatilized $^{14}\text{CO}_2$ and volatile [^{14}C]organic compounds totaled 0.5% and 0.3% of the applied, respectively.

Transformation pathways consistent with the products detected in this study were provided by the study authors. Major pathways include formation of M800H08 from saflufenacil through

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reduction of the double bond of the uracil ring, M800H01 through demethylation of parent at the nitrogen of the isopropyl amino group, and M800H02 through demethylation of parent at the uracil nitrogen. Minor pathways include cleavage of the uracil ring to form M800H07 or M800H15-ketohydrate. Further cleavage of M800H07 yields trifluoroacetic acid, while uracil ring cleavage of M800H08 yields M800H22. Post-flooding, rates of degradation of parent saflufenacil and formation of products were both significantly slowed, with residues diffusing from the soil into the water layer at a ratio of *ca.* 3:1 (water:soil). Formation of bound soil residues remained low ($\leq 7.5\%$ of applied) throughout the study, with minimal formation of CO_2 or volatile organics (each $\leq 0.5\%$ of applied).

Results Synopsis:

Test system used: Loamy sand soil from Wisconsin.

Half-life/DT50 values post-flood (reviewer-calculated).

Non-linear SFO DT50 in water:	ND (insufficient dissipation; both labels).
Non-linear SFO DT50 in soil:	19.5 days ($r^2 = 0.8042$; [Phenyl-U- ^{14}C]-label).
	7.0 days ($r^2 = 0.8503$; [Uracil-4- ^{14}C]-label).
	11.3 days ($r^2 = 0.8148$; combined labels).
Non-linear SFO DT50 in total system:	217 days (combined labels).
Non-linear SFO DT90 in total system:	721 days (combined labels).

Products detected post-flooding:

Major transformation products:

- N³-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-tetrahydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide (M800H08; maximum 20.0%, 7.5% and 25.4% of applied in water layer, soil and total system, respectively).
- N³-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropylsulfamide (M800H01; maximum 11.0% of applied in both water layer and soil, 14.9% in total system).
- N³-[2-chloro-4-fluoro-5-(2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)-4-fluorobenzoyl]-N-isopropyl-N-methylsulfamide (M800H02; maximum 18.5%, 4.6% and 24.0% of applied in water layer, soil and total system, respectively).

Minor transformation products:

- N-{4-chloro-2-fluoro-5-[(isopropyl(methyl)amino)-sulfonyl]amino)carbonyl]phenyl}-4,4,4-trifluoro-3,3-dihydroxybutanamide (M800H15-ketohydrate; maximum 1.6%, 1.2% and 1.9% of applied in water layer, soil and total system, respectively).
- 3-[(4-chloro-2-fluoro-5-[(isopropyl(methyl)amino)-sulfonyl]amino)carbonyl]aniline(methyl)amino]-4,4,4-trifluorobutanoic acid (M800H22; 1.6% of applied in water layer and total system, 0.4% in soil).
- N-{4-chloro-2-fluoro-5-[(isopropyl(methyl)amino)-sulfonyl]amino)carbonyl]phenyl}-N³-methylurea (M800H07; maximum 3.3%, 1.3% and 4.4% of applied in water layer, soil and total system, respectively).
- Trifluoroacetic acid (maximum 3.4%, 1.0% and 4.0% of applied in water layer, soil and total system, respectively).

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CO₂ (maximum 0.5% of applied).
Volatile organics (maximum 0.3% of applied).

Study Acceptability: This study is classified as **supplemental/reliable with restrictions**. No deviations from good scientific practices were noted. During the anaerobic phase of the study, anaerobic conditions were marginal.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with USEPA Subdivision N Guideline §162-2 (pp. 22, 38). The following significant deviation from the objectives of Subdivision N guidelines that may affect the interpretation of the study results was noted:

During the anaerobic phase of the study, anaerobic conditions were marginal.

COMPLIANCE: This study was conducted in compliance with USEPA GLP Standards (40 CFR Part 160) with the exception that the study protocol was not made available to Agvise Laboratories during the soil characterization (p. 3). Signed and dated Data Confidentiality, GLP, Quality Assurance, and [study] Certification statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Materials

[Phenyl-U-¹⁴C]- and [uracil-4-¹⁴C]-labeled saflufenacil (pp. 14-15).

Chemical Structure:

See DER Attachment 1.

Phenyl label

Description:

Technical, solid (pp. 14, 19).

Purity: Radiochemical purity:

≥95% via HPLC (pp. 14-15, 19-20, 28; Figure 5, p. 57; Figure 7, p. 59).

Lot/Batch No.:

825-1501 (p. 14).

Analytical purity:

Not reported.

Specific activity:

279,000 dpm/μg (4.65 MBq/mg, p. 14).

Location of the radiolabel:

Uniformly on phenyl ring (p. 14).

Uracil label

Description:

Technical, in acetonitrile (pp. 15, 19).

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Purity: Radiochemical purity: $\geq 98\%$ via HPLC (pp. 15, 19-20, 28; Figure 4, p. 56; Figure 6, p. 58).
Lot/Batch No.: 829-1201 (p. 15).
Analytical purity: Not reported.
Specific activity: 248,400 dpm/ μ g (4.14 MBq/mg, p. 15).
Location of the radiolabel: At 4-C of uracil ring (p. 15).

Storage conditions of test chemicals: The test substances and reference compounds were stored frozen (0 to -30°C ; pp. 16, 19).

Physico-chemical properties of saflufenacil:¹

Parameter		Value	Comment
Molecular weight (g/Mol)		500.86	
Molecular formula		$\text{C}_{17}\text{H}_{17}\text{ClF}_4\text{N}_4\text{O}_5\text{S}$	
Water solubility (mg/L)	pH 4, 20°C :	14 (pH 4, 20°C)	
	pH 5, 20°C :	25 (pH 5, 20°C)	
	pH 7, 20°C :	2100 (pH 7, 20°C)	
	pH 9, 20°C :	Not determined due to degradation.	
Vapor pressure	20°C :	4.5×10^{-15} Pa	Indicates nonvolatility.
	25°C :	2.0×10^{-14} Pa	
UV Absorption	pH 1, pH 7:	UV/VIS $\lambda_{\text{max}} = 272$ nm	Indicates possible susceptibility to direct photolysis at alkaline pH.
	pH 12:	UV/VIS $\lambda_{\text{max}} = 309$ nm	
pKa		4.41	Indicates neutrality at ambient pH.
K_{ow}		368	Indicates low potential to bioconcentrate.
$\log K_{\text{ow}}$		2.56	
Stability of compound at room temperature		Stable for >2 yrs.	

Data obtained from Genari, 2007 (MRID 47127814); Beery, 2007 (MRID 47127815); Beery, 2006 (MRID 47127817); Vanhook, 2005 (MRID 47127818); Vanhook, 2005a (MRID 47127819); and Kroel, 2005 (MRID 47127821).

¹ Solubility in water and pKa values provided in the study report were inconsistent with the submitted product chemistry data.

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2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description	Details
Geographic location	Buffalo County, Wisconsin.
Pesticide use history at the collection site	Not reported.
Collection date	May 13, 2008.
Collection procedures	Not reported.
Sampling depth	Not reported.
Storage conditions	Collected soil was received at the test facility on May 16, 2008, where the soil was stored refrigerated (1-10°C) until use. Conditions during transfer from the collection site to the test facility were not reported.
Storage length	42 days prior to preparation of test systems for acclimatization.
Soil preparation	The test soil was 2-mm sieved prior to use. Six days prior to treatment (June 24, 2008), aliquots (50 g dry wt.) of soil were transferred to 125-mL Nalgene polypropylene containers and maintained in darkness at $25 \pm 1^\circ\text{C}$, with continuous aeration initiated 5 days prior to treatment.

Data obtained from pp. 20-21 of the study report.

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Table 2: Properties of the soil.

Property	Details
Soil texture ¹	Loamy sand.
% Sand (50-2,000 µm)	85
% Silt (2-50 µm)	11
% Clay (<2 µm)	4
pH in soil:water (1:1)	6.0
Organic carbon (%) ²	0.9
Organic matter (%)	1.5
CEC (meq/100 g)	7.6
Moisture at 1/3 bar (%)	6.9
Bulk density, disturbed (g/cm ³)	1.33
Microbial biomass (µg C/g dry wt)	87.4
Soil series (USDA)	Plainfield.
Soil taxonomic classification	Mixed, mesic typic, Udipsamment.
Sol mapping unit	Not reported.

Data obtained from p. 12; Table 1, p. 40 of the study report.

- 1 The particle size scale was not specified; however, the textural classification was performed by AGVISE Laboratories, Northwood, North Dakota (p. 12), who reported a USDA textural class. Therefore, USDA particle size scales were likely to have been used.
- 2 Determined using the following formula: organic carbon (%) = organic matter (%) / 1.72.

B. EXPERIMENTAL CONDITIONS:

1. **Preliminary experiments:** No preliminary experiments were described.

2. **Experimental conditions:**

Table 3: Experimental design.

Parameter			Details	
Duration of the test (posttreatment)			92 days; 17 days of aerobic incubation followed by 75 days of anaerobic incubation.	
Soil condition: (Air dried/fresh)			Fresh.	
Soil (g/replicate)			50 g dry wt. (53.7 ± 0.1 g wet wt., layer depth <i>ca.</i> 2.6-2.9 cm).	
Application rate (mg a.i./kg & equiv. kg a.i./ha)	Nominal:		1.06 mg a.i./kg (1.20 kg a.i./ha ¹); 53 µg [¹⁴ C]saflufenacil/50 g dry wt. soil.	
	Actual:	Phenyl-label:	1.07 mg a.i./kg (53.7373 µg a.i./50 g dry wt. soil).	
		Uracil-label:	1.12 mg a.i./kg (56.1494 µg a.i./50 g dry wt. soil).	
Control conditions, if used			No sterile controls were prepared.	
No. of Replications	Controls, if used		No sterile controls were prepared.	
	Treatment		For each label, twenty-two samples were treated with	

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Parameter		Details
		[¹⁴ C]saflufenacil to allow for duplicate replicates at each of eleven sampling intervals (single replicates).
Test apparatus	Type/material/volume	125-mL Nalgene polypropylene containers connected to a flow-through volatiles trapping system. Treated systems were connected in series (sample trains); two series, each having eleven treated systems, per label. The layout of the test apparatus is illustrated in Figure 3, p. 55. <u>Aerobic phase</u> : continuous CO ₂ -free air (flow rate not reported). <u>Anaerobic phase</u> : continuous humidified nitrogen gas (flow rate not reported) at 0-6 and 15-75 days post-flooding, with the systems maintained sealed (capped) at 6-14 days post-flooding.
	Details of traps for CO ₂ and volatile organics, if any	<u>Aerobic phase</u> : 0.5N NaOH (two traps, volumes not reported) to trap CO ₂ . The volatile trapping apparatus is illustrated in Figure 3, p. 55. <u>Anaerobic phase</u> : at 0-6 days post-flooding, 0.5N NaOH (two traps, volumes not reported) to trap CO ₂ . Then at 15-75 days post-flooding, ethylene glycol (one trap, volume not reported) to trap volatile organics and 0.5N NaOH (one trap, volume not reported) to trap CO ₂ . Volatiles were not collected at 6-14 days post-flooding.
If no traps were used, is the system closed/open?		Continuous flow-through volatiles trapping systems were used, except when the systems were maintained sealed at 6-14 days post-flooding.
Identity and concentration of co-solvent		Acetonitrile; final concentration 0.4% based on soil dry wt..
Test material application method	Volume of the test solution used/treatment:	200 µL.
	Application method:	Test solution applied to soil surface with a VWR microdispenser.
	Is the co-solvent evaporated?	Not reported.
Any indication of the test material adsorbing to the walls of the test apparatus?		Not reported.
Microbial biomass/population of sterile controls (units)		No sterile controls were prepared.
Microbial biomass/population of treated soil (units)		Treated soil was not analyzed for microbial biomass.
Experimental conditions:	Temperature (°C):	25 ± 1°C.
	Continuous darkness (Yes/No):	Yes.
	Moisture content:	<u>Aerobic phase</u> : 99% of water holding capacity at 1/3 bar (6.8% soil moisture). <u>Anaerobic phase</u> : treated soil flooded with 100 mL (depth from container bottom to water surface <i>ca.</i> 6.5-6.7 cm) of dextrose-amended (0.1% wt.:vol. dextrose monohydrate powder) bottled water (Burdick and Jackson High Purity Solvent) after 17 days of aerobic incubation.

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Parameter		Details
	Moisture maintenance method:	<u>Aerobic phase</u> : soil moisture was adjusted to 99% of water holding capacity at 1/3 bar gravimetrically just prior to treatment and at 10 days posttreatment. <u>Anaerobic phase</u> : nitrogen flow was directed through a container of water.
Other details, if any		Aliquots (0.5-1 mL) of 10-20% (wt.:vol) dextrose solution, final concentration 0.1% based on water volume, were added at 28 and 48 days post-flooding to help maintain anaerobic conditions. For each label, a single untreated system was prepared and incubated with (attached in series) the treated systems.

Data obtained from pp. 6, 19-23, 29; Table 2, p. 41; Tables 4-5, pp. 43-44; Figure 3, p. 55 of the study report.

1 Based on conversion factor 1 mg a.i./kg = 1.13 kg a.i./ha.

3. Aerobic/anaerobic conditions: Following treatment, the soil samples were incubated aerobically under a continuous-flow (flow rate not reported), CO₂-free air atmosphere (p. 21; Figure 3, p. 55). The treated soil samples were converted to anaerobic conditions after 17 days of aerobic incubation by flooding the soil with dextrose-amended (0.1% wt.:vol), high-purity bottled water (100 mL) and changing the flow-through gas to humidified nitrogen (pp. 22-23). During 75 days of anaerobic incubation, the incubation vessels were continuously flushed with humidified nitrogen gas (flow rate not reported), except at 6-14 days post-flooding when the systems were maintained sealed (capped) under static conditions (p. 23; Table 2, p. 41). At 6 days post-flooding (initial post-flood interval, 23 days posttreatment) in untreated systems, redox potentials and dissolved oxygen in the water layer were -213 to -11 mV (n = 2) and 0.25 mg/L (n = 1), respectively (Table 2, p. 41).

4. Supplementary experiments: Metabolite identification (10x High Dose) systems. Four soil samples were treated with [uracil-4-¹⁴C]saflufenacil combined with [uracil-5-¹³C, benzamide carbonyl-¹³C]saflufenacil (purity 98.87%, radiochemical purity >96%, Lot No.: 828-1085) [¹⁴C:¹³C ratio 15:85] at 10 mg a.i./L (500 µg a.i./50g dry wt. soil) and incubated under the same conditions as the 1x treated systems (pp. 15, 21, 29, 33; Figure 24, p. 76). Water-soil systems were taken for analysis at 91 days post-flooding (p. 33). No additional details regarding incubation conditions and/or sampling were provided.

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5. Sampling:

Table 4: Sampling details.

Criteria	Details
Sampling intervals (days posttreatment)	0, 14, 17, 23, 28, 35, 43, 51, 59, 77 and 92.
Sampling method	For each label, duplicate treated samples were taken at each collection interval, except at 23 and 43 days posttreatment (6 and 26 days post-flooding) when a single treated system per label was collected.
Method of collection of CO ₂ and organic volatile compounds	Trapping solutions were collected and replaced at 14, 17, 23, 35, 43, 51, 59, 77 and 92 days posttreatment; however, volatiles collection was not employed at 23-31 days posttreatment (6-14 days post-flooding).
Sampling intervals/times for: Sterility check, if sterile controls are used: Moisture content: Dissolved oxygen at water-soil interface, pH in water layer and redox potential in soil:	No sterile controls were prepared. During aerobic incubation, soil moisture was adjusted just prior to treatment and at 10 days posttreatment, 7 days prior to flooding. Measured in untreated systems at first post-flood interval (6 days post-flooding, 23 days posttreatment) and in treated systems at all remaining post-flood intervals (11-75 days post-flooding, 28-92 days posttreatment).
Sample storage before analysis	Soil and water layer, when present, were separated the day of collection, and the soil extracted within two days of sampling. Water layers and soil extracts were stored refrigerated (1-10°C) prior to analysis. Trapping solutions (NaOH, ethylene glycol) were stored at room temperature. Water layers, soil extracts and trapping solutions were analyzed by LSC within two days of sampling. Water layers and soil extracts were analyzed by HPLC within 28 days of sample collection.
Other observation, if any	None.

Data obtained from pp. 22-24, 27, 29; Table 2, p. 41; Tables 4-5, pp. 43-44; Appendix 1, pp. 80-81 of the study report.

C. ANALYTICAL METHODS:

Separation of the water and soil: The water layer, when present, was separated from the soil by centrifugation (*ca.* 2,500-3,600 rpm, 10-20 minutes) and decanted (p. 24). Triplicate aliquots (0.1 mL) were analyzed for total radioactivity by LSC (p. 24; Appendix 2, p. 82).

Extraction/clean up/concentration methods: Water layers were analyzed directly (p. 24).

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Soil was extracted once with acetonitrile, followed by twice with acetonitrile:water (70:30, v:v); extraction solvent volumes were 100 mL (p. 22; Figure 8, p. 60). Each extraction was done via shaking (*ca.* 300 rpm, mechanism not specified) for 30 minutes; after which, soil and extract were separated via centrifugation (*ca.* 2,500-3,600 rpm, 15-20 minutes; p. 24). Extracts were analyzed for total radioactivity by LSC (triplicate aliquots, volume not reported), then combined and concentrated *in vacuo* and via N-Evap for chromatographic analysis (p. 24). Recoveries following concentration of soil extracts were reported as >90% (p. 31); individual recoveries were not reported.

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the water layers (when present), soil extracts, extracted soil and volatile trapping solutions (Tables 4-5, pp. 43-44).

Determination of non-extractable residues: Extracted soil was air-dried and ground to homogenize (mechanism not specified), then triplicate aliquots (weight not reported) were analyzed for total radioactivity by LSC following combustion (pp. 24-25).

Determination of volatile residues: Triplicate aliquots of the NaOH (1 mL) and ethylene glycol (volume not reported) trapping solutions were analyzed for total radioactivity by LSC (p. 24; Appendix 2, p. 83).

Derivatization method, if used: None was reported.

Identification and quantification of parent compound: Water layers and soil extracts were analyzed by reverse-phase HPLC under the following conditions (method BAS800A2): Waters YMC ODS-AQ column (4.6 x 250 mm, 5 μm), gradient mobile phase combining (A) 0.5% aqueous formic acid and (B) acetonitrile [percent A:B at 0.0-6.0 min. 90:10 (v:v), 36.0-38.0 min. 10:90, 38.5-40.0 min. 90:10], flow rate 1 mL/minute, UV diode-array detector (254 nm), IN/US BetaRam radioactivity detector equipped with a 200- μL solid-flow cell (p. 25). Selected column recoveries averaged $99 \pm 8\%$ (range 88-111%, $n = 5$); all column recoveries were not reported (p. 26). Parent [^{14}C]saflufenacil was identified by comparison to the retention time of unlabeled reference standard (p. 25; Table 8, p. 51; Figures 1-2, pp. 53-54; Figure 9, p. 61; Figures 11-18, pp. 63-70).

To confirm identification, parent [^{14}C]:[^{13}C]saflufenacil was isolated via HPLC fraction collection from a concentrated 91-day post-flood high-dose water layer sample; details regarding concentration of the water layer sample and conditions during fraction collection were not reported (p. 33; Figure 20, p. 72). Isolated parent [^{14}C]:[^{13}C]saflufenacil (Lab0422) was analyzed by LC/MS and LC/MS/MS under the following conditions: Phenomenex Columbus LC column (2.0 x 100 mm, 5 μm), gradient mobile phase combining (A) 0.1% formic acid in water:methanol (98:2, v:v) and (B) 0.1% formic acid in methanol:water (98:2, v:v) [percent A:B at 0.0 min. 98:2 (v:v), 10.0-20.0 min. 2:98, 20.1-25.0 min. 98:2], flow rate 0.3 mL/minute, IN/US BetaRam radioactivity detector, Thermo Scientific LCQ DECA MS, electrospray

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ionization (ESI), positive ion mode, full scan (pp. 33-34; Appendix 4, pp. 86-89). Isolated [¹⁴C]:[¹³C]saflufenacil was identified against labeled reference standard (pp. 33-34; Appendix 4, pp. 88-89, 94-96).

Identification and quantification of transformation products: Transformation products were separated and quantified using HPLC as described for the parent compound (p. 25; Table 8, p. 51; Figures 1-2, pp. 53-54; Figure 9, p. 61; Figures 13-18, pp. 65-70; Figures 25-26, pp. 77-78).

In an attempt to better resolve transformation products, M800H22 and M800H02, the HPLC gradient mobile phase was modified as follows (method BAS800A3): [percent A:B at 0.0-2.0 min. 90:10 (v:v), 36.0-38.0 min. 10:90, 38.5-40.0 min. 90:10]; however, since only very low levels of product M800H22 were detected, this method was not used for quantitation (p. 25).

Transformation products M800H08 (Lab0423), M800H02 (Lab0425) and M800H01 (Lab0424) were isolated via HPLC fraction collection from a concentrated 91-day post-flood high-dose water layer sample and analyzed by LC/MS and LC/MS/MS as described above (pp. 34-35; Figures 21-23, pp. 73-75; Appendix 4, pp. 86-93, 97-107).

Table 5: Reference compounds available for identifying transformation products of saflufenacil.

Applicant Code (Registry Number)	Chemical Name	Purity ¹	Lot/Batch No.
M800H01 (4118561)	N'-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropylsulfamide	98.8%	L74-62
M800H02 (4118416)	N'-[2-chloro-4-fluoro-5-(2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)-4-fluorobenzoyl]-N-isopropyl-N-methylsulfamide	99.2%	L67-186
M800H07 (4775453)	N-{4-chloro-2-fluoro-5-[[{[(isopropyl(methyl)amino)sulfonyl]-amino}carbonyl]phenyl]-N'-methylurea	95.4%	L67-196
M800H08 (4773881)	N'-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-tetrahydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide	97.2%	L74-66
M800H15-ketohydrate (5264357)	N-{4-chloro-2-fluoro-5-[[{[(isopropyl(methyl)amino)sulfonyl]-amino}carbonyl]phenyl]-4,4,4-trifluoro-3,3-dihydroxybutanamide	94.5%	L74-80
M800H22 (5216337)	3-[(4-chloro-2-fluoro-5-[[{[(isopropyl(methyl)amino)sulfonyl]amino}carbonyl]anilino}carbonyl](methyl)amino)-4,4,4-trifluorobutanoic acid	94.1%	L74-56
None (207584)	[1- ¹⁴ C]-labeled trifluoroacetic acid, sodium salt	99.8% ²	ARC-1079

Data obtained from pp. 16-19 of the study report.

1 Purity w/w unless otherwise designated.

2 Radiochemical purity via HPLC as acid.

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Detection limits (LOD, LOQ) for the parent compound and transformation products: For HPLC analyses, the limit of detection (LOD) was reported as a signal:noise ratio of 2:1 for the radioactivity detector (p. 26). Limits of quantitation (LOQ) were reported as low as 0.03587 μg (10,008 dpm, amount injected) for a [phenyl-U- ^{14}C]-label treated water sample, but were more typically 0.071-0.105 μg (19,905-29,209 dpm) for [phenyl-U- ^{14}C]-label treated samples and 0.0711-0.132 μg (17,671-32,689 dpm) for [uracil-4- ^{14}C]-label treated samples [p. 26; Figure 9, p. 61 (Figure 9 is incorrectly titled as [uracil-4- ^{14}C]-label treated)].

For LSC analyses, the LOD was reported as *ca.* 60 dpm (100 dpm prior to subtraction of background radioactivity) or *ca.* 2×10^{-4} μg (equivalent to *ca.* 0.0004% of the applied for [uracil-4- ^{14}C]-label treated samples), with a LOQ of $\geq 0.004\% \pm \leq 10\%$ (p. 25).

II. RESULTS AND DISCUSSION

For [phenyl-U- ^{14}C]-label treated soil, air-flow to the Replicate 2 sample series (train) was reportedly greater than to the Replicate 1 sample series due to a malfunctioning manifold (pp. 22, 29; Figure 3, p. 55). The study authors believed that moisture levels of the Replicate 2 treated soil samples in the vessels closest to the air entry were impacted to the point that soil metabolic activity was significantly decreased in the Replicate 2 systems collected at 35-92 days posttreatment (18-75 days post-flooding). Consequently, the study authors did not use results from the 35- to 92-day [phenyl-U- ^{14}C]-label treated Replicate 2 samples to determine mean levels of parent saflufenacil and its transformation products or in kinetic evaluations. However, the reviewer deemed that the results, though divergent, did not alter the overall conclusions drawn from the study and included the results in all calculations.

A. TEST CONDITIONS: During the 75-day incubation post-flooding, conditions in the soil layers (both labels) were reducing (-200 to -50 mV) to moderately reducing (-50 to +200 mV) with an average redox potential of -34 ± 88 mV (range -224 to +113 mV, $n = 28$; Table 6; DER Attachment II). Dissolved oxygen at the water-soil interface averaged 0.16 ± 0.04 mg/L (0.11-0.25 mg/L, $n = 26$), while water layer pH levels averaged 5.3 ± 0.3 (5.0-6.0, $n = 28$, measured only with pH paper). The incubation temperature was reportedly maintained at $25 \pm 1^\circ\text{C}$ throughout the study, except during a 24-hour interval at 49-50 days posttreatment when the temperature increased to 26.4°C ; no supporting temperature records were provided (pp. 20, 28).

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Table 6: Treated system parameters (pH, O₂ and redox potentials).

Day ¹	[Phenyl-U- ¹⁴ C]-label			[Uracil-4- ¹⁴ C]-label		
	Water	Interface	Soil	Water	Interface	Soil
	pH ²	O ₂ (mg/L)	Redox (mV)	pH ²	O ₂ (mg/L)	Redox (mV)
23	5.0	0.25	-213	5.0	(no report)	-11
28	5.0	0.25	113	5.0	0.22	-55
	5.0	0.24	102	5.0	0.25	97
35	5.0	0.15	25	5.0	(no report)	49
	5.0	0.14	28	5.0	0.15	18
43	5.5	0.13	-3	5.5	0.13	-1
51	5.5	0.13	-73	5.5	0.13	-218
	5.5	0.11	-224	5.5	0.13	-213
57	5.5	0.14	-6	5.0	0.13	-30
	5.5	0.13	-34	5.5	0.14	-15
77	5.0	0.15	-21	5.5	0.14	-36
	5.5	0.15	-18	5.0	0.14	-31
92	5.5	0.14	-30	5.5	0.14	-36
	6.0	0.15	-85	5.5	0.14	-27

Results from Table 2, p. 41 of the study report.

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

2 Determined using pH paper (p. 24 of the study report).

B. MATERIAL BALANCE: Overall recovery of radiolabeled material (labels combined) averaged $98.5 \pm 2.2\%$ (range 92.6-105.6%, n = 40) of the applied, with no pattern of decline in recoveries over the 92-day incubation for either label (DER Attachment 2, Reviewer's Comment No. 1). For each label, recoveries averaged (n = 20) $98.2 \pm 2.8\%$ (range 92.6-105.6%) and $98.9 \pm 1.3\%$ (range 96.0-100.9%) for the [phenyl-U-¹⁴C]- and [uracil-4-¹⁴C]-label treated systems, respectively.

After flooding at 17 days posttreatment, [¹⁴C]residues readily partitioned from the soil to the water layer with distribution ratios (water:soil, either n = 1 or mean, n = 2) of 2:1 at 6-26 days post-flood (23-43 days posttreatment) and 3:1 at 34-75 post-flood (51-92 days posttreatment) for the [phenyl-U-¹⁴C]-label treated systems, and 2:1 at 6 days post-flood and 3:1 at 11-75 days post-flood for the [uracil-4-¹⁴C]-label treated systems (DER Attachment 2).

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Table 7: Biotransformation of [phenyl-U-¹⁴C]saflufenacil (BAS 800 H), expressed as percentage of applied radioactivity (n = 1¹), in Wisconsin loamy sand soil under anaerobic conditions.

Compound		Sampling times (days posttreatment)										
		Aerobic			Anaerobic							
		0	14	17	23	28	35	43	51	59	77	92
Saflufenacil	Water	NA ²	NA	NA	21.5	19.4	19.4	-- ⁶	22.4	19.4	21.4	20.8
	Soil	93.8	47.5	36.8	10.1	8.4	7.3	--	6.2	6.5	6.7	5.3
	System	NA	NA	NA	31.6	27.8	26.7	--	28.6	25.9	30.1	26.1
M800H08	Water	NA	NA	NA	10.1	15.7	18.7	--	12.2	14.2	14.4	14.1
	Soil	ND ³	15.8	17.5	4.5	7.5	6.4	--	3.4	3.8	4.5	3.4
	System	NA	NA	NA	14.6	23.2	25.1	--	15.6	18.0	18.9	17.5
M800H01	Water	NA	NA	NA	9.4	8.7	9.3	--	11.0	9.8	7.5	8.2
	Soil	ND	14.1	11.6	3.2	2.3	2.4	--	2.5	2.0	2.0	1.8
	System	NA	NA	NA	12.6	11.0	11.7	--	13.5	11.8	9.5	10.0
M800H02	Water	NA	NA	NA	12.8	11.8	13.7	-	16.3	15.2	17.2	19.8
	Soil	ND	18.0	14.6	3.6	4.1	4.0	--	4.0	4.2	4.5	4.2
	System	NA	NA	NA	16.4	15.9	17.7	--	20.3	19.4	21.7	24.0
M800H07	Water	NA	NA	NA	2.6	2.5	2.5	--	2.1	2.8	3.3	1.3
	Soil	ND	1.8	1.5	0.9	1.2	1.0	--	0.9	1.1	1.1	0.2
	System	NA	NA	NA	3.5	3.7	3.5	--	3.0	3.9	4.4	1.5
M800H15-ketohydrate	Water	NA	NA	NA	0.8	1.1	ND	ND	ND	ND	0.9	ND
	Soil	ND	1.3	1.1	ND	0.4	ND	--	ND	ND	ND	0.2
	System	NA	NA	NA	0.8	1.5	ND	ND	ND	ND	0.9	0.2
M800H22	Soil ⁴	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.3	0.2
Unidentified [¹⁴ C]residues ⁵	Water	NA	NA	NA	5.0	3.9	5.3	--	3.1	7.4	5.4	4.6
	Soil	2.1	7.5	5.0	1.7	1.4	2.9	--	2.6	2.1	2.1	3.5
	System	NA	NA	NA	6.7	5.3	8.2	--	5.7	9.5	7.5	8.1
Extractable soil residues		99.5	93.8	90.1	26.8	25.0	24.0	--	21.9	22.6	21.0	20.0

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Table 7: Biotransformation of [phenyl-U-¹⁴C]saflufenacil (BAS 800 H), expressed as percentage of applied radioactivity (n = 1¹), in Wisconsin loamy sand soil under anaerobic conditions.

Compound		Sampling times (days posttreatment)										
		Aerobic			Anaerobic							
		0	14	17	23	28	35	43	51	59	77	92
Nonextractable soil residues		0.5	5.8	6.3	4.8	5.0	5.3	--	4.4	5.2	5.8	5.5
CO ₂		--	0.1	0.1	0.1	--	0.1	0.1	0.1	0.1	0.1	0.1
Volatile organics		--	--	--	--	--	ND	ND	ND	ND	ND	ND
Total recovery	Water	NA	NA	NA	63.9	65.2	70.9		71.8	70.8	71.5	73.1
	Soil	100.0	99.6	96.4	31.6	30.0	29.3	--	26.3	27.8	26.8	25.5
	System	100.0	99.7	96.5	95.6	95.2	100.3	--	98.2	98.7	98.4	98.7

1 Only data from replicate 1 were reported by the reviewer because data from replicate 2 were invalid (Table 4, p. 43; Table 6, pp. 45-47; DER Attachment 2).

2 Not applicable, soil flooded at 17 days posttreatment.

3 Not detected.

4 Detected only in soil extracts.

5 Consisting of three unknowns (UNK 25.8 min., UNK 26.3 min., UNK 26.6 min.) plus "Other" intermittently detected residues, with no individual component detected at >3.9% of the applied in the water layer, >4.0% in soil extracts, or >4.9% in the total system (Table 6, p. 47; DER Attachment 2).

6 Not collected.

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EPA MRID Number 47611201

PMRA Submission Number 2008-0431

Table 8: Biotransformation of [uracil-4-¹⁴C]saflufenacil (BAS 800 H), expressed as percentage of applied radioactivity (either n = 1, or mean ± s.d., n = 2¹), in Wisconsin loamy sand soil under anaerobic conditions.

Compound		Sampling times (days posttreatment)										
		Aerobic			Anaerobic							
		0	14	17	23	28	35	43	51	59	77	92
Saflufenacil	Water	NA ²	NA	NA	31.1	28.8 ± 0.3	29.4 ± 1.5	28.7	27.8 ± 0.1	27.0 ± 0.3	25.7 ± 0.1	26.8 ± 1.0
	Soil	114 ± 3	49.8 ± 4.1	44.3 ± 4.0	12.3	9.7 ± 1.8	10.7 ± 0.4	10.0	8.3 ± 1.3	8.8 ± 2.6	8.0 ± 0.8	8.3 ± 0.3
	System	NA	NA	NA	43.4	38.5 ± 1.4	40.1 ± 1.9	38.7	36.0 ± 1.2	35.7 ± 2.2	33.7 ± 0.8	35.1 ± 0.8
M800H08	Water	NA	NA	NA	10.1	13.0 ± 4.5	14.8 ± 1.1	13.7	14.4 ± 0.4	16.8 ± 1.3	16.9 ± 1.6	16.0 ± 2.5
	Soil	ND ³	14.1 ± 0.9	14.6 ± 2.8	4.4	4.7 ± 0.5	5.5 ± 0.3	4.7	4.6 ± 1.0	4.5 ± 1.2	5.6 ± 0.1	4.7 ± 0.3
	System	NA	NA	NA	14.5	17.7 ± 5.0	20.3 ± 1.4	18.4	19.0 ± 1.4	21.2 ± 0.1	22.5 ± 1.5	20.7 ± 2.8
M800H01	Water	NA	NA	NA	7.4	8.0 ± 1.5	8.0 ± 0.5	9.4	7.8 ± 0.9	8.5 ± 0.3	8.6 ± 0.6	9.1 ± 1.2
	Soil	ND	10.7 ± 1.7	10.6 ± 0.7	2.3	1.8 ± 0.4	2.4 ± 0.2	2.3	2.1 ± 0.5	1.9 ± 0.5	2.2 ± 0.0	2.0 ± 0.0
	System	NA	NA	NA	9.7	9.8 ± 1.9	10.4 ± 0.7	11.7	9.9 ± 1.4	10.3 ± 0.2	10.7 ± 0.6	11.1 ± 1.2
M800H02	Water	NA	NA	NA	13.0	15.6 ± 0.6	12.6 ± 2.8	10.4	15.3 ± 3.2	14.3 ± 3.7	13.7 ± 0.4	15.5 ± 1.6
	Soil	ND	10.5 ± 2.1	13.2 ± 1.2	2.8	3.8 ± 0.8	3.7 ± 0.9	2.9	4.0 ± 0.1	3.5 ± 0.1	3.7 ± 0.5	3.7 ± 0.6
	System	NA	NA	NA	15.8	19.3 ± 1.3	16.3 ± 3.7	13.3	19.3 ± 3.3	17.8 ± 3.6	17.4 ± 0.8	19.2 ± 2.2
M800H15-ketohydrate	Water	NA	NA	NA	1.2	0.9 ± 0.0	1.6, ND	ND	ND	ND	ND	ND
	Soil	ND	ND, 1.7	ND	ND	ND	0.3, ND	0.3	1.1 ± 0.2	0.4 ± 0.2	ND, 0.2	ND
	System	NA	NA	NA	1.2	0.9 ± 0.0	1.9, ND	0.3	1.1 ± 0.2	0.4 ± 0.2	ND, 0.2	ND
M800H22	Water	NA	NA	NA	ND	ND	ND	ND	ND	ND	1.6 ± 0.0	ND
	Soil	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.2 ± 0.0
	System	NA	NA	NA	ND	ND	ND	ND	ND	ND	1.6 ± 0.0	0.2 ± 0.0
Trifluoroacetic acid	Water	NA	NA	NA	2.6	2.6 ± 0.7	ND, 3.1	2.4	2.5 ± 0.2	1.6 ± 0.1	3.1 ± 0.4	2.2 ± 0.6
	Soil	ND	2.7 ± 0.0	5.9 ± 1.1	ND	0.5, ND	ND	ND	ND, 0.8	0.9 ± 0.1	0.7 ± 0.1	0.9 ± 0.0
	System	NA	NA	NA	2.6	2.8 ± 0.4	ND, 3.1	2.4	2.9 ± 0.6	2.5 ± 0.2	3.7 ± 0.3	3.1 ± 0.6
Unidentified [¹⁴ C]residues ⁴	Water	NA	NA	NA	4.2	4.7 ± 0.8	5.8 ± 1.6	10.1	5.7 ± 2.1	5.3 ± 1.3	2.6 ± 0.8	5.7 ± 1.8
	Soil	ND	3.7 ± 0.6	3.8 ± 0.0	0.8	1.2 ± 0.4	1.1 ± 0.3	2.1	2.0 ± 0.3	1.9 ± 0.0	1.3 ± 0.3	0.8 ± 0.2

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Table 8: Biotransformation of [uracil-4-¹⁴C]saflufenacil (BAS 800 H), expressed as percentage of applied radioactivity (either n = 1, or mean ± s.d., n = 2¹), in Wisconsin loamy sand soil under anaerobic conditions.

Compound		Sampling times (days posttreatment)										
		Aerobic			Anaerobic							
		0	14	17	23	28	35	43	51	59	77	92
	System	NA	NA	NA	5.0	5.9 ± 1.2	6.8 ± 1.3	12.2	7.7 ± 2.4	7.2 ± 1.4	3.9 ± 0.6	6.5 ± 2.0
Extractable soil residues		100.1 ± 0.3	92.7 ± 0.9	93.1 ± 1.6	25.1	21.2 ± 1.8	22.6 ± 0.7	21.2	21.0 ± 2.2	21.9 ± 3.6	21.3 ± 0.1	20.1 ± 0.6
Nonextractable soil residues		0.3 ± 0.0	4.9 ± 0.5	5.3 ± 0.5	3.5	3.5 ± 0.0	3.7 ± 0.2	3.4	3.8 ± 0.2	3.9 ± 0.6	4.0 ± 0.2	3.8 ± 0.0
CO ₂		-- ⁵	0.1 ± 0.0	0.2 ± 0.1	0.2 ± 0.1	--	0.2 ± 0.0	0.3 ± 0.1	0.3 ± 0.1	0.4 ± 0.1	0.4 ± 0.1	0.5 ± 0.1
Volatile organics		--	--	--	--	--	ND	ND	0.1 ± 0.0	0.2 ± 0.1	0.2 ± 0.1	0.3 ± 0.1
Total recovery	Water	NA	NA	NA	69.7	73.4 ± 1.2	72.8 ± 0.3	74.9	73.4 ± 0.1	73.2 ± 4.2	73.1 ± 1.6	74.9 ± 0.9
	Soil	100.4 ± 0.3	97.6 ± 1.4	98.3 ± 1.2	28.6	24.7 ± 1.8	26.2 ± 0.9	24.6	24.8 ± 2.4	25.8 ± 4.2	25.2 ± 0.0	23.8 ± 0.5
	System	100.4 ± 0.3	97.7 ± 1.4	98.5 ± 1.3	98.5	98.1 ± 0.6	99.2 ± 0.7	99.7	98.5 ± 2.5	99.6 ± 0.2	98.9 ± 1.3	99.4 ± 0.3

1 Means and standard deviations calculated by the reviewer using data obtained from Table 5, p. 44; Table 7, pp. 48-50 (DER Attachment 2).

2 Not applicable, soil flooded at 17 days posttreatment.

3 Not detected.

4 Consisting of three unknowns (UNK 25.8 min., UNK 26.3 min., UNK 26.6 min.) plus "Other" intermittently detected residues, with no individual component detected at >4.5% of the applied in the water layer and total system, or >4.3% in soil extracts (Table 7, p. 50; DER Attachment 2).

5 Not collected.

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C. TRANSFORMATION OF PARENT COMPOUND: Flooding significantly slowed the overall rate of degradation with [^{14}C]saflufenacil (both labels) in the soil decreasing from 93.8-117% of the applied at day 0 posttreatment to 36.8-48.2% at 17 days, just prior to flooding, then post-flooding was 31.6-43.4% in the total system at 23 days posttreatment (6 days post-flood) and 26.1-37.8% at 92 days (75 days post-flood, DER Attachment 2). In the water and soil post-flooding, [^{14}C]saflufenacil (both labels) was 21.5-31.1% and 10.1-12.3% of the applied, respectively, at 23 days posttreatment (6 days post-flood) slowly decreasing to 20.8-30.5% and 5.3-8.5%, respectively, at 92 days (75 days post-flood).

HALF-LIFE/DT50/DT90: Reviewer-observed DT50 (50% decline time) values for saflufenacil (both labels) were <6 days post-flooding in the soil and >75 days post-flooding in the water layer and total system, with reviewer-observed DT90 (90% decline time) values of >75 days post-flooding in the water, soil and total system. Reviewer-calculated half-lives were not determined for saflufenacil in the water layers and total systems due to insufficient dissipation post-flooding. First-order linear regression analysis (Excel 2007) yielded half-lives for [phenyl- ^{14}C] - and [uracil-4- ^{14}C]-labeled saflufenacil of 46 and 49 days, respectively, in the soil (all replicates, all post-flood intervals), with respective nonlinear (SigmaPlot v 9.0) half-lives of 20 and 7 days (DER Attachment 2). Comparison of the [phenyl- ^{14}C]-labeled Replicate 1 (moisture maintained) and Replicate 2 (drier) soil samples determined linear half-lives of 44 and 43 days, respectively, with respective nonlinear half-lives of 5 and 25 days.

The study authors determined DT50, DT75 and DT90 values for saflufenacil (labels combined) in the total system (flooded soil) of 228, 456 and 757 days, respectively, using single first-order nonlinear (two-compartment) analysis ($r^2 = 0.193$), and DT50, DT75 and DT90 values for saflufenacil in the aerobic and anaerobic (flooded) soil of 12.6, 215 and 808 days using double first-order nonlinear (two-compartment) analysis ($r^2 = 0.949$, ModelMaker v 4.0; p. 36; Appendix 5, pp. 111-123). For both analyses, results from the 35- to 92-day Replicate 2 [phenyl- ^{14}C]-label treated systems were not included in the calculations because the study authors believed the decreased levels of degradation of parent saflufenacil in those systems were a consequence of lowered soil moisture during the aerobic incubation (p. 36). These values were not confirmed by the reviewer.

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Half-lives/DT50/DT90 post-flooding

Phase	Half-life/DT50 ¹ (days post-flooding)	Regression equation	r ²	Observed DT50 ² (days)	Observed DT90 ² (days)
[Phenyl-U- ¹⁴ C]-label					
Water (Replicates 1 and 2)					
Linear/natural log	ND ³	--	--	>75	>75
Nonlinear/normal	ND ³	--	--		
Loamy sand soil (Replicates 1 and 2)					
Linear/natural log	45.7	y = -0.0152x + 2.9386	0.3755	<6	>75
Nonlinear/normal	19.5	y = 30.1exp(-0.0355x)	0.8042		
Loamy sand soil (Replicate 1 samples)					
Linear/natural log	44.4	y = -0.0156x + 2.6429	0.4664	<6	>75
Nonlinear/normal	4.7	y = 35.6exp(-0.1489x)	0.8863		
Loamy sand soil (Replicate 2 samples)					
Linear/natural log	43.3	y = -0.0160x + 3.2775	0.6271	<6	>75
Nonlinear/normal	24.5	y = 35.8exp(-0.0283x)	0.8973		
Total system (Replicates 1 and 2)					
Linear/natural log	ND ³	--	--	>75	>75
Nonlinear/normal	ND ³	--	--		
[Uracil-4- ¹⁴ C]-label					
Water (Replicates 1 and 2)					
Linear/natural log	ND ³	--	--	>75	>75
Nonlinear/normal	ND ³	--	--		
Loamy sand soil (Replicates 1 and 2)					
Linear/natural log	49.2	y = -0.0141x + 2.8528	0.3807	<6	>75
Nonlinear/normal	7.0	y = 41.2exp(-0.0985x)	0.8503		
Total system (Replicates 1 and 2)					
Linear/natural log	ND ³	--	--	>75	>75
Nonlinear/normal	ND ³	--	--		
Labels combined					
Water (all Replicates)					
Linear/natural log	ND ³	--	--	>75	>75
Nonlinear/normal	ND ³	--	--		
Loamy sand soil (all Replicates)					
Linear/natural log	47.4	y = -0.0146x + 2.8957	0.3767	<6	>75
Nonlinear/normal	11.3	y = 35.7exp(-0.0612x)	0.8148		
Total system (all Replicates)					
Linear/natural log	ND ³	--	--	>75	>75
Nonlinear/normal	217 (DT90 721)	--	--		

1 Determined by the reviewer using Excel 2007 (linear, first-order) and SigmaPlot v 9.0 (nonlinear, one-compartment/two-parameter) and sample data obtained from Table 6, p. 45; Table 7, p. 48 of the study report (DER Attachment 2).

2 Reviewer-observed DT50 and DT90 values; based on mean [¹⁴C]saflufenacil detected, when applicable.

3 Not determined due to insufficient dissipation of saflufenacil.

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TRANSFORMATION PRODUCTS: Three major nonvolatile transformation products,

- N'-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-tetrahydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide (M800H08),
- N'-[2-chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropylsulfamide (M800H01), and
- N'-[2-chloro-4-fluoro-5-(2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)-4-fluorobenzoyl]-N-isopropyl-N-methylsulfamide (M800H02), and

two minor products,

- N-{4-chloro-2-fluoro-5-[[[(isopropyl(methyl)amino)sulfonyl]amino]carbonyl]phenyl}-4,4,4-trifluoro-3,3-dihydroxybutanamide (M800H15-ketohydrate) and
- 3-[[[(4-chloro-2-fluoro-5-[[[(isopropyl(methyl)amino)sulfonyl]amino]carbonyl]aniline)carbonyl](methyl)amino]-4,4,4-trifluorobutanoic acid (M800H22),

were detected with both labels, while minor product

- N-{4-chloro-2-fluoro-5-[[[(isopropyl(methyl)amino)sulfonyl]amino]carbonyl]phenyl}-N'-methylurea (M800H07)

was detected only in [phenyl-U-¹⁴C]-label treated samples and minor product

- trifluoroacetic acid

was detected only in [uracil-4-¹⁴C]-label treated samples. Major products M800H08, M800H01 and M800H02 were isolated from a 91-day high dose [uracil-4-¹⁴C]:[uracil-5-¹³C, benzamide carbonyl-¹³C]saflufenacil-treated water layer sample and identifications confirmed via LC/MS and LC/MS/MS against reference standards (pp. 34-35; Figures 21-23, pp. 73-75; Appendix 4, pp. 87, 89-93, 97-108). Identifications of minor products were made by comparison to HPLC retention times of reference standards (Figures 1-2, pp. 53-54; Figures 13-18, pp. 65-70; Figures 25-26, pp. 77-78).

[Phenyl-U-¹⁴C]saflufenacil treated soil. M800H08 was 15.8-20.2% of the applied in the soil at 14-17 days posttreatment, then post-flooding was 14.6% in the total system (10.1% water layer, 4.5% soil) at 23 days (6 days post-flood), 14.1-25.1% (10.3-18.7% water layer, 3.8-7.5% soil) at 28-35 days (11-18 days post-flood) and 17.5-25.4% (14.1-20.0% water layer, 3.4-5.4% soil) at 92 days (75 days post-flood, DER Attachment 2). M800H01 was 7.5-14.1% in the soil at 14-17 days posttreatment, then post-flooding was 12.6% in the total system (9.4% water layer, 3.2% soil) at 23 days (6 days post-flood) and 7.1-10.0% (5.8-8.2% water layer, 1.3-1.8% soil) at 92 days (75 days post-flood). M800H02 was 5.4-18.0% in the soil at 14-17 days posttreatment, then post-flooding was 16.4% in the total system (12.8% water layer, 3.6% soil) at 23 days (6

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days post-flood) and 9.6-24.0% (8.3-19.8% water layer, 1.3-4.2% soil) at 92 days (75 days post-flood). M800H07 was a maximum 3.7% in the soil at 17 days, then post-flooding was maximums of 3.3%, 1.3% and 4.4% in the water, soil and total system, respectively. M800H15-ketohydrate was a maximum 2.3% in the soil at 14 days, then post-flooding was maximums of 1.1%, 0.5% and 1.5% in the water layer, soil and total system, respectively. M800H22 was detected only in the soil post-flooding at $\leq 0.4\%$. Total unidentified [^{14}C]residues, comprised of several components, were detected at maximums of 7.5% in the water layer and soil and 9.5% in the total system, with no individual component detected at $>3.9\%$, 4.0% or 4.9% in the water layer, soil or total system, respectively.

[Uracil-4- ^{14}C]saflufenacil treated soil. M800H08 was 11.8-17.4% of the applied in the soil at 14-17 days posttreatment, then post-flooding was 14.5% in the total system (10.1% water layer, 4.4% soil) at 23 days (6 days post-flood), 12.7-22.6% (8.5-18.0% water layer, 3.3-5.8% soil) at 28-59 days (11-42 days post-flood), 21.0-23.9% (15.3-18.5% water layer, 5.4-5.7% soil) at 77 days (60 days post-flood) and 17.9-23.5% (13.5-18.5% water layer, 4.4-5.0% soil) at 92 days (75 days post-flood, DER Attachment 2). M800H01 was 9.0-12.3% in the soil at 14-17 days posttreatment, then post-flooding was 9.7% in the total system (7.4% water layer, 2.3% soil) at 23 days (6 days post-flood) and 9.9-12.2% (7.9-10.3% water layer, 1.9-2.0% soil) at 92 days (75 days post-flood). M800H02 was 8.4-14.4% in the soil at 14-17 days posttreatment, then post-flooding was 15.8% in the total system (13.0% water layer, 2.8% soil) at 23 days (6 days post-flood), 12.6-22.5% (9.8-18.5% water layer, 2.8-4.6% soil) at 28-77 days (11-60 days post-flood) and 17.0-21.3% (13.9-17.0% water layer, 3.1-4.3% soil) at 92 days (75 days post-flood). M800H15-ketohydrate was a maximum 1.7% in the soil at 14 days, then post-flooding was maximums of 1.6%, 1.2% and 1.9% in the water layer, soil and total system, respectively. M800H22 was detected only post-flooding at maximums of 1.6% in the water and total system and 0.2% in the soil. Trifluoroacetic acid was a maximum 6.9% in the soil at 17 days, then post-flooding was maximums of 3.4%, 1.0% and 4.0% in the water layer, soil and total system, respectively. Total unidentified [^{14}C]residues, comprised of several components, were detected at maximums of 10.1%, 4.3% and 12.2% in the water layer, soil and total system, respectively, with no individual component detected at $>4.5\%$ in the water layer and total system, or $>4.3\%$ in the soil.

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: [Phenyl-U- ^{14}C]saflufenacil treated soil. Extractable soil [^{14}C]residues were 99.5% (n = 2) of the applied at day 0 and 88.7-93.8% at 14-17 days, then post-flooding gradually decreased from 26.8% at 23 days (6 days post-flood) to 19.8-20.0% at 92 days (75 days post-flood, DER Attachment 2). Nonextractable soil [^{14}C]residues were 0.5% (n = 2) of the applied at day 0 and 3.5-7.5% at 14-92 days.

[Uracil-4- ^{14}C]saflufenacil treated soil. Extractable soil [^{14}C]residues were 99.7-100.4% of the applied at day 0 and 91.4-94.7% at 14-17 days, then post-flooding were 25.1% at 23 days (6 days post-flood) and 19.5-20.6% at 92 days (75 days post-flood, DER Attachment 2). Nonextractable soil [^{14}C]residues were 0.3% (n = 2) of the applied at day 0 and 3.3-5.7% at 14-92 days.

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VOLATILIZATION: At study termination (92 days) for both labels, volatilized $^{14}\text{CO}_2$ and volatile [^{14}C]organic compounds totaled $\leq 0.5\%$ and $\leq 0.3\%$ of the applied, respectively (DER Attachment 2).

TRANSFORMATION PATHWAY: The study authors provided transformation pathways that were consistent with the transformation products detected in this study (pp. 36-37; Figure 27, p. 79). Major pathways include formation of M800H08 from saflufenacil through reduction of the double bond of the uracil ring, M800H01 through demethylation of parent at the nitrogen of the isopropyl amino group, and M800H02 through demethylation of parent at the uracil nitrogen. Minor pathways include cleavage of the uracil ring to form M800H07 or M800H15-ketohydrate. Further cleavage of M800H07 yields trifluoroacetic acid, while uracil ring cleavage of M800H08 yields M800H22. Post-flooding, rates of degradation of parent saflufenacil and formation of products were both significantly slowed, with residues diffusing from the soil into the water layer at a ratio of *ca.* 3:1 (water:soil). For both labels, three minor unknowns ($R_t = 25.8$ min., 26.3 min. and 26.6 min.) were detected post-flooding; each detected at $< 5\%$ of applied in the total system. Formation of bound soil residues remained low ($\leq 7.5\%$ of applied) throughout the study, with minimal formation of CO_2 or volatile organics (each $\leq 0.5\%$ of applied).

Table 9: Chemical names and CAS numbers for the transformation products of saflufenacil.

Applicant Code (Registry No.)	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
M800H01 (4118561)	None	N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)-benzoyl]-N-isopropylsulfamide	$\text{C}_{16}\text{H}_{15}\text{ClF}_4\text{N}_4\text{O}_5\text{S}$	486.83	-- ¹
M800H02 (4118416)	None	N'-[2-Chloro-4-fluoro-5-(2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)-4-fluorobenzoyl]-N-isopropyl-N-methylsulfamide	$\text{C}_{16}\text{H}_{15}\text{ClF}_4\text{N}_4\text{O}_5\text{S}$	486.83	--
M800H07 (4775453)	None	N-{4-Chloro-2-fluoro-5-[[[(isopropyl(methyl)-amino)sulfonyl]amino]carbonyl]phenyl}-N'-methylurea	$\text{C}_{13}\text{H}_{18}\text{ClFN}_4\text{O}_4\text{S}$	380.83	--
M800H08 (4773881)	None	N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-tetrahydro-1(2H)-pyrimidinyl)-benzoyl]-N-isopropyl-N-methylsulfamide	$\text{C}_{17}\text{H}_{19}\text{ClF}_4\text{N}_4\text{O}_5\text{S}$	502.87	--
M800H15- ketohydrate (5264357)	None	N-{4-Chloro-2-fluoro-5-[[[(isopropyl(methyl)-amino)sulfonyl]amino]carbonyl]phenyl}-4,4,4-trifluoro-3,3-dihydroxybutanamide	$\text{C}_{15}\text{H}_{18}\text{ClF}_4\text{N}_3\text{O}_6\text{S}$	479.84	--
M800H22 (5216337)	None	3-[(4-Chloro-2-fluoro-5-[[[(isopropyl(methyl)amino]-sulfonyl)amino]-carbonyl]anilino]carbonyl(methyl)amino]-4,4,4-trifluorobutanoic acid	$\text{C}_{17}\text{H}_{21}\text{ClF}_4\text{N}_4\text{O}_6\text{S}$	520.89	--
Trifluoroacetic acid	--	Trifluoroacetic acid	$\text{C}_2\text{HF}_3\text{O}_2$ ³	114	--

Information from pp. 16-19; Table 8, p. 51 of the study report.

1 Information not provided.

2 The molecular formula provided by the study authors was incorrect and that of M800H07 (pp. 16, 18).

3 Chemical formula determined from provided structure (Table 8, p. 51).

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PMRA Submission Number 2008-0431

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D. SUPPLEMENTARY EXPERIMENT-RESULTS: Storage stability. Reanalysis of a 35-day (18-day post-flood) water layer sample after 1 month of refrigerated storage showed a product profile quantitatively similar to the initial analysis (p. 28; Figure 19, p. 71).

Metabolite identification (10x High Dose) systems. Parent saflufenacil and the major transformation products, M800H08, M800H01 and M800H02, were isolated from 91-day high dose [uracil-4-¹⁴C]:[uracil-5-¹³C, benzamide carbonyl-¹³C]saflufenacil-treated water layer sample and identifications confirmed via LC/MS and LC/MS/MS against reference standards, as described above (pp. 33-35; Figures 20-23, pp. 72-75; Appendix 4, pp. 86-108).

III. STUDY DEFICIENCIES

1. Anaerobic conditions were marginal during the anaerobic phase of the study. Although oxygen levels remained low throughout the study, soil redox potential was rarely less than -100mV (range -224 to +113 mV). However, efforts were made (*e.g.*, addition of dextrose and resumption of nitrogen flow) to correct this. Also, flooding significantly slowed the overall rate of degradation of saflufenacil in the soil, indicating that a change of conditions consistent with anaerobicity had occurred after the flooding took place. Given the study conditions were not definitively anaerobic, the study classification is downgraded.
2. For phenyl-label treated soil, air-flow to the Replicate 2 sample series (train) was greater than to the Replicate 1 sample series due to a malfunctioning manifold (pp. 22, 29; Figure 3, p. 55). The study authors believed that moisture levels of the Replicate 2 treated soil samples in the vessels closest to the air entry were impacted to the point that soil metabolic activity was significantly decreased in the Replicate 2 systems collected at 35-92 days posttreatment (18-75 days post-flooding). At 35-77 days posttreatment (18-60 days post-flood), levels of parent saflufenacil in the total system of the phenyl-label treated Replicate 2 samples were *ca.* 2-3x greater as compared to the Replicate 1 samples. The study authors provided the results from the 35- to 92-day phenyl-label treated Replicate 2 samples, but did not use those results to determine mean levels of parent saflufenacil and its transformation products or in kinetic evaluations. The reviewer excluded data from this replicate in its entirety from kinetics calculations. This deficiency does not affect the acceptability of the study.
3. The reported level of quantitation for LSC was unreasonably vague ($\geq 0.004\% \pm \leq 10\%$). This deficiency does not affect the acceptability of the study.

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IV. REVIEWER'S COMMENTS

1. During the aerobic incubation interval, soil moisture was adjusted gravimetrically to 99% of water-holding capacity just prior to treatment and at 10 days posttreatment (7 days prior to flooding), rather than at 75% of 1/3 bar.
2. All mean results and standard deviations presented in this review were determined by the primary reviewer using Microsoft Excel 2007 (12.0.6024.5000) MSO (12.0.6017.5000) software (DER Attachment 2). Standard deviations were determined using the "biased" or "n" method which determines the standard deviation of the entire sample population. Material balance summations, summations of total saflufenacil and its products in the total system and mean results, excluding mean results for unidentified residues, reported by the study authors (Tables 4-7, pp. 43-50) were verified by the primary reviewer and, with the exceptions noted below, there was consistent agreement (within $\pm 0.1\%$ of applied) between the study authors' reported mean values and those determined by the primary reviewer (DER Attachment 2).

Calculation discrepancies:

- Material balances determined by the primary reviewer for phenyl-label treated systems at day 17 (Rep 1, Rep 2), day 43 (Rep 2), day 51 (Rep 1) and day 77 (Rep 1, Rep 2) differed by 0.2-0.3% from the results reported by the study authors, possibly due to rounding differences (DER Attachment 2).
- Material balances determined by the primary reviewer for uracil-label treated systems at day 17 (Rep 1), day 23 (Rep 1), day 35 (Rep 1) and days 43-92 (all Reps) differed by 0.2-0.8% from the results reported by the study authors. At the later intervals, it appears volatilized residues were not included in the material balances reported in the study (DER Attachment 2).
- For the 92-day Rep 2 phenyl-label treated system, the primary reviewer determined M800H02 comprised 9.6% of applied in the total system, whereas the study authors reported 7.6% (Table 6, p. 46; DER Attachment 2).
- For the 92-day Rep 2 uracil-label treated system, the primary reviewer determined parent saflufenacil comprised 35.8% of applied in the total system, whereas the study authors reported 38.5% (Table 7, p. 48; DER Attachment 2).
- For the 35-day Rep 1 uracil-label treated system, the primary reviewer determined M800H15-ketohydrate comprised 1.9% of applied in the total system, whereas the study authors reported 1.6%; this appears to be a summation error (Table 7, p. 49; DER Attachment 2).

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- Four other instances of total systems discrepancies occurred with UNK 25.8 min in uracil-label treated Rep 1 systems at 23 and 92 days, and with UNK 26.3 min in uracil-label treated Rep 1 and 2 systems at 51 days (Table 7, pp. 48-49; DER Attachment 2).

Typographical errors:

- Table 3 (p. 42), ethylene glycol traps were not utilized at the 23-day (6-day post-flood) interval (p. 23).
 - Figure 9 (p. 61), the figure titled indicates analysis of a water sample from a uracil-label treated system, when the system was phenyl-label treated.
3. Aqueous solubilities of saflufenacil at 20°C were reported in the study report as 3.6 mg/L at pH 2, 119 mg/L at pH 5, and 936.6 mg/L at pH 7 and the pKa was reported as 4.3 (p. 14). These values disagree with those of the referenced product chemistry studies (p. 37).
 4. The test soil for this study was collected from the same site from which soil was collected for use in an aerobic soil metabolism study (Singh, 2007; MRID 47445901; pp. 20, 38).
 5. The test application rate of 53 µg/50 g dry wt. soil selected for this study was reported as equivalent to the maximum yearly application rate for saflufenacil in forestry use of 0.36 lb a.i./A (400 g a.i./ha, p. 21). However, the test application rate is three-fold higher (1,200 g a.i./ha) than the maximum yearly application rate, using the common conversion factor 1 mg a.i./kg = 1.13 kg a.i./ha.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-2, Anaerobic Soil Metabolism Studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.
2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

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Attachment 1: Structures of Parent Compound and Transformation Products

Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

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PMRA Submission Number 2008-0431

EPA MRID Number 47611201

Saflufenacil [BAS 800 H, BAS800H, BAS 800H, CL No. 433379, 4054449, AC 433,379]

IUPAC Name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

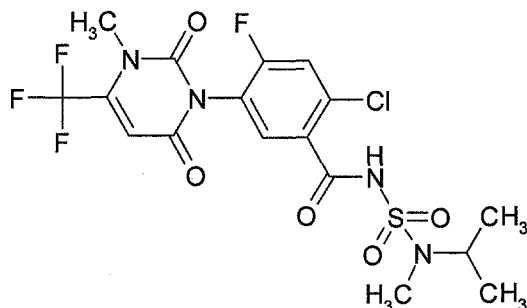
CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

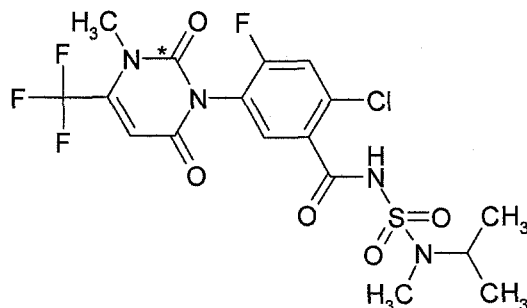
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Empirical formula: C₁₇H₁₇ClF₄N₄O₅S **Molecular formula:** C₁₇H₁₇ClF₄N₄O₅S

Unlabeled



[Uracil-4-¹⁴C]Saflufenacil



* = Location of the radiolabel.

Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

PMRA Document Number 1686946
PMRA Submission Number 2008-0431

EPA MRID Number 47611201

Saflufenacil [BAS 800 H, BAS800H, BAS 800H, CL No. 433379, 4054449, AC 433,379]

IUPAC Name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

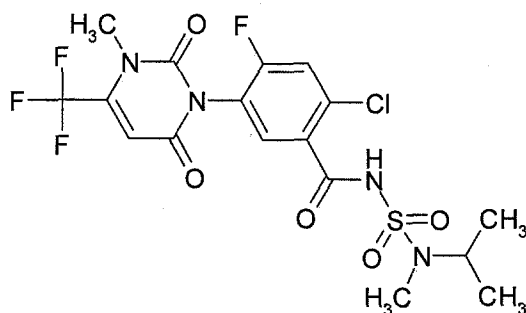
CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

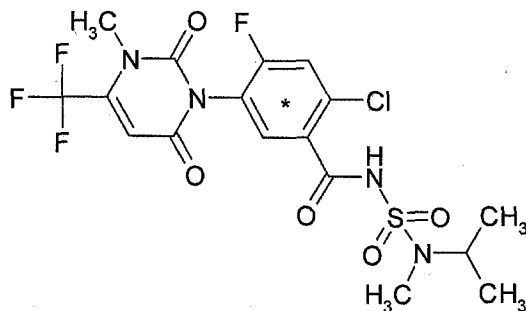
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Empirical formula: C₁₇H₁₇ClF₄N₄O₅S **Molecular formula:** C₁₇H₁₇ClF₄N₄O₅S

Unlabeled



[Phenyl-U-¹⁴C]Saflufenacil



* = Location of the radiolabel.

Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

PMRA Document Number 1686946

EPA MRID Number 47611201

PMRA Submission Number 2008-0431

Identified Compounds

Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

PMRA Document Number 1686946
PMRA Submission Number 2008-0431

EPA MRID Number 47611201

Saflufenacil [BAS 800 H, BAS800H, BAS 800H, CL No. 433379, 4054449, AC 433,379]

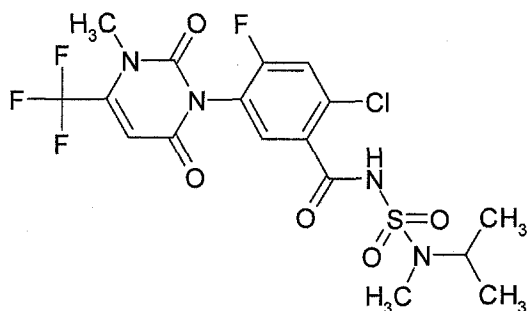
IUPAC Name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

SMILES String: N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(C)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

Empirical formula: C₁₇H₁₇ClF₄N₄O₅S **Molecular formula:** C₁₇H₁₇ClF₄N₄O₅S

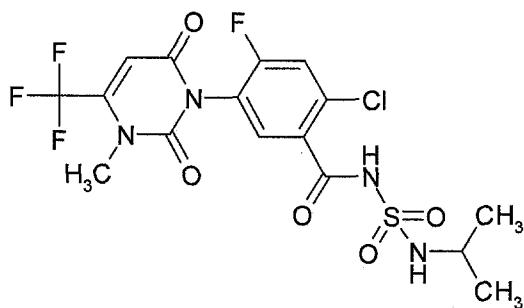


M800H01 [4118561]

IUPAC Name: N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N'-isopropylsulfamide.

CAS Name: Not reported.

CAS Number: Not reported.



Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

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PMRA Submission Number 2008-0431

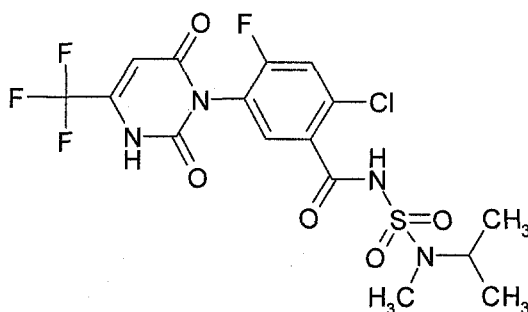
EPA MRID Number 47611201

M800H02 [4118416]

IUPAC Name: N'-[2-Chloro-5-(2,6-dioxo-4-(trifluoromethyl)-3,6-dihydropyrimidin-1(2H)-yl)-4-fluorobenzoyl]-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-5-(2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)-4-fluorobenzoyl]-N-isopropyl-N-methylsulfamide.

CAS Name: Not reported.

CAS Number: Not reported.

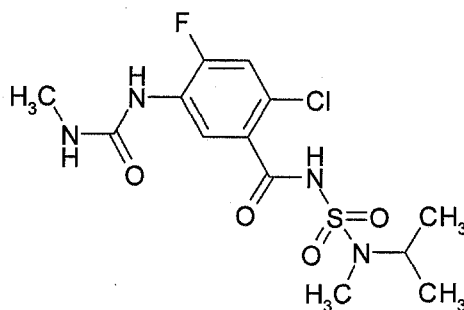


M800H07 [4775453]

IUPAC Name: N-{4-Chloro-2-fluoro-5-[[[isopropyl(methyl)amino]sulfonyl]amino]carbonyl]phenyl}-N'-methylurea.

CAS Name: Not reported.

CAS Number: Not reported.



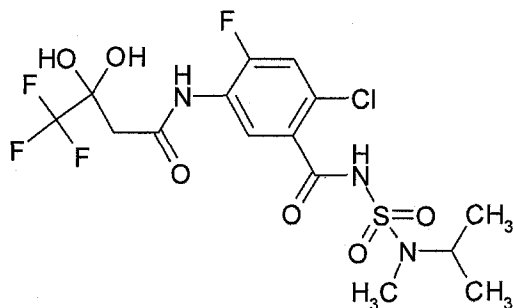
Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

PMRA Document Number 1686946
PMRA Submission Number 2008-0431

EPA MRID Number 47611201

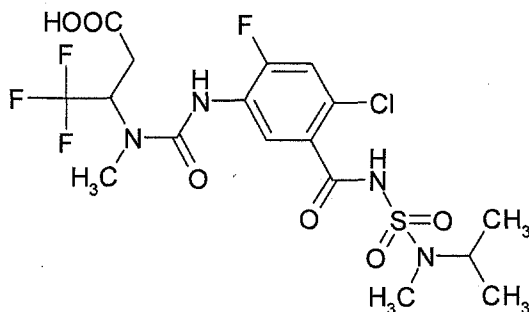
M800H15 [M800H15-ketohydrate, "Ketohydrate", 5264357]

IUPAC Name: N-{4-Chloro-2-fluoro-5-
[[([isopropyl(methyl)amino)sulfonyl]amino)carbonyl]phenyl}-4-4-4-
trifluoro-3,3-dihydroxybutanamide.
CAS Name: Not reported.
CAS Number: Not reported.



M800H22 [5216337]

IUPAC Name: 3-[(4-Chloro-2-fluoro-5-
[[([isopropyl(methyl)amino)sulfonyl]amino)carbonyl]anilino}carbonyl)(methyl)amino]-4,4,4-trifluorobutanoic acid.
CAS Name: Not reported.
CAS Number: Not reported.



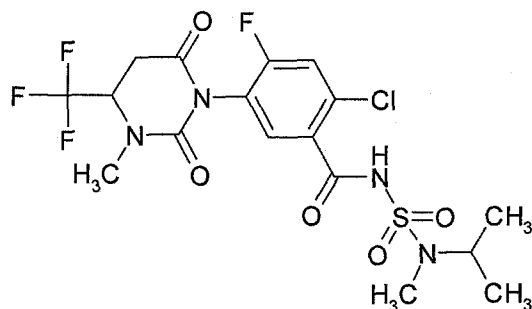
Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

PMRA Document Number 1686946
PMRA Submission Number 2008-0431

EPA MRID Number 47611201

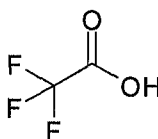
M800H08 [4773881]

IUPAC Name: N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)tetrahydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.
CAS Name: Not reported.
CAS Number: Not reported.



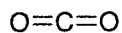
TFA [M800H29]

IUPAC Name: Trifluoroacetic acid.
CAS Name: Not reported.
CAS Number: Not reported.



Carbon Dioxide

IUPAC Name: Carbon dioxide.
CAS Name: Carbon dioxide.
CAS Number: 124-38-9.



Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

PMRA Document Number 1686946

EPA MRID Number 47611201

PMRA Submission Number 2008-0431

Unidentified Reference Compounds

Data Evaluation Record on the anaerobic biotransformation of saflufenacil (BAS 800 H) in soil

PMRA Document Number 1686946
PMRA Submission Number 2008-0431

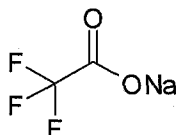
EPA MRID Number 47611201

Trifluoroacetic acid, sodium salt [207584, TF acetic acid]

IUPAC Name: Trifluoroacetic acid, sodium salt.

CAS Name: Not reported.

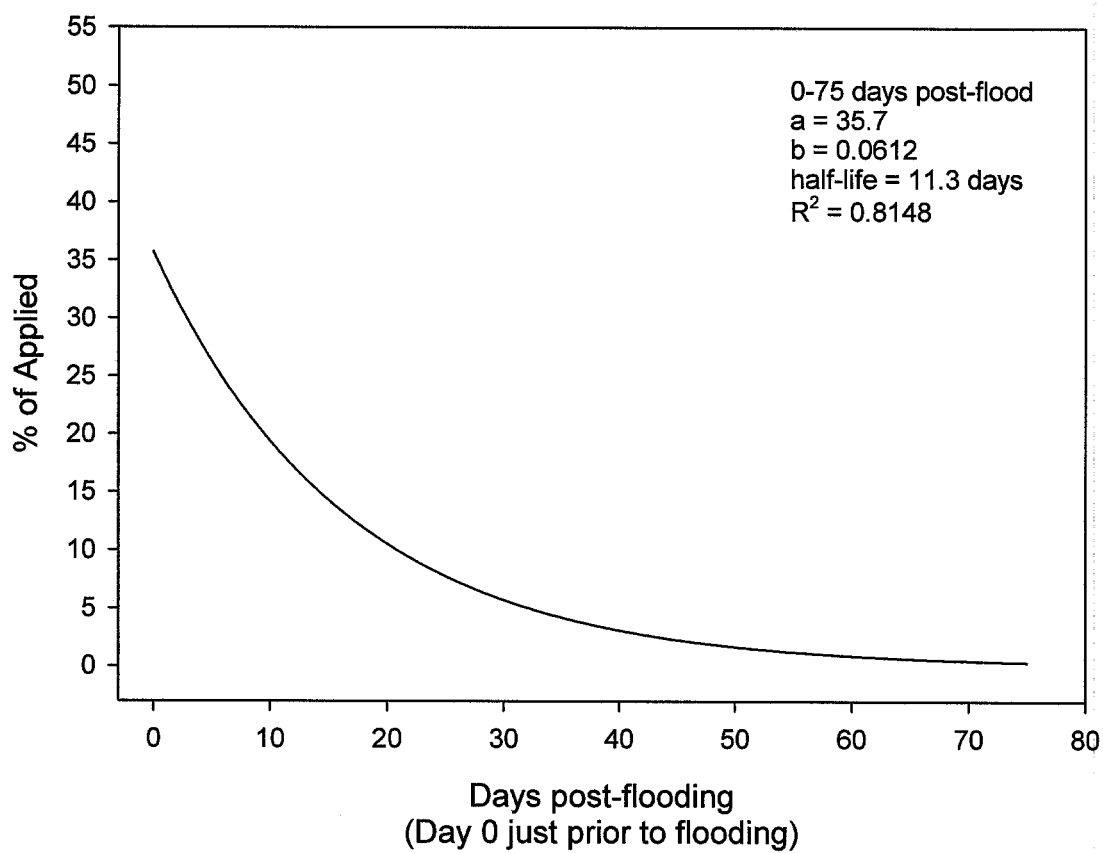
CAS Number: Not reported.



Attachment 2: Excel and SigmaPlot Spreadsheets

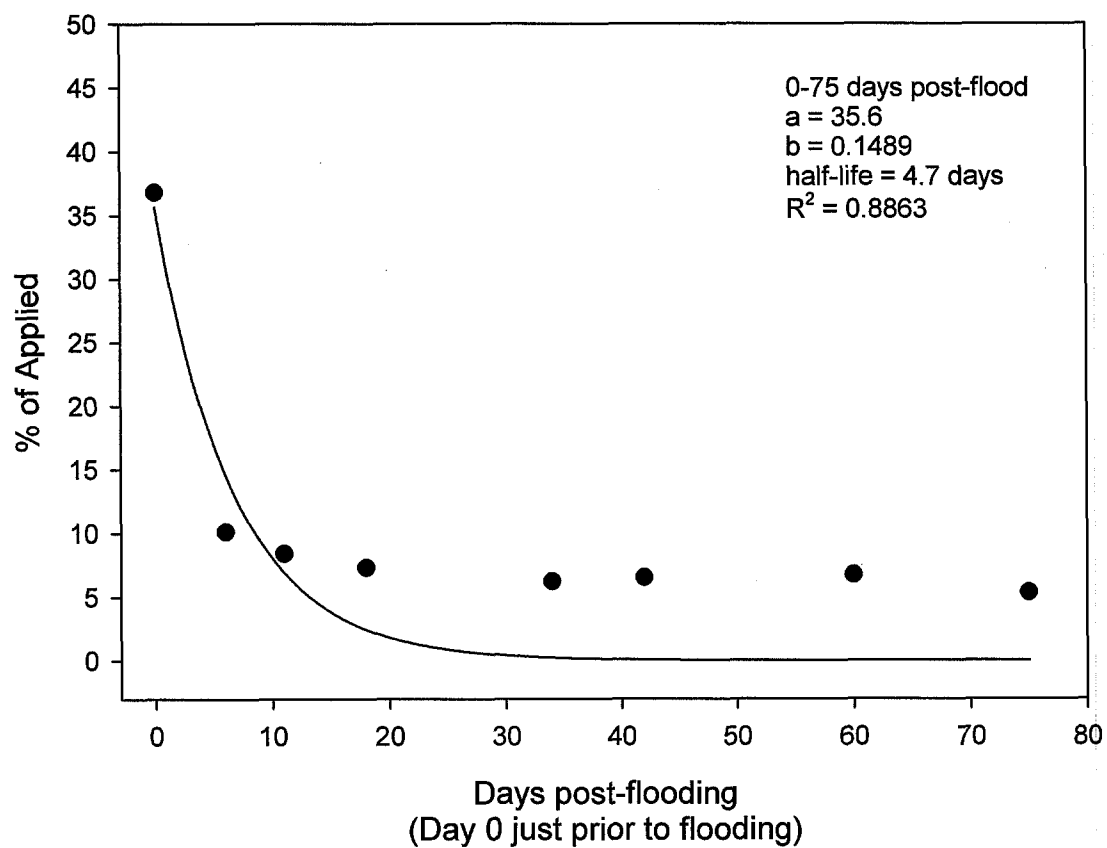
Chemical: Saflufenacil (BAS 800 H)
PC: 118203
MRID: 47611201
Guideline: 835.4200

[¹⁴C]Saflufenacil in anaerobic Wisconsin
loamy sand soil: soil, labels combined (1/2 model, nonlinear)



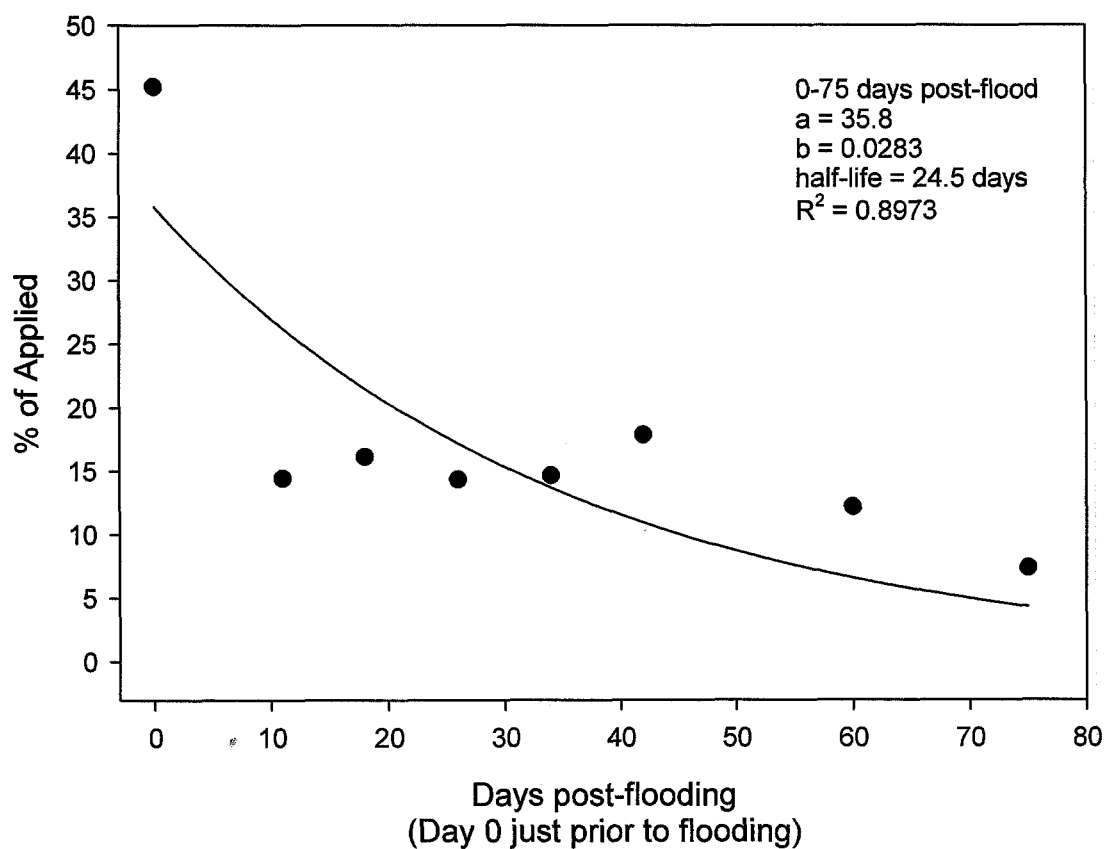
Chemical: Saflufenacil (BAS 800 H)
PC: 118203
MRID: 47611201
Guideline: 835.4200

[Phenyl-U-¹⁴C]saflufenacil in anaerobic Wisconsin
loamy sand soil: soil Rep 1 samples (1/2 model, nonlinear)



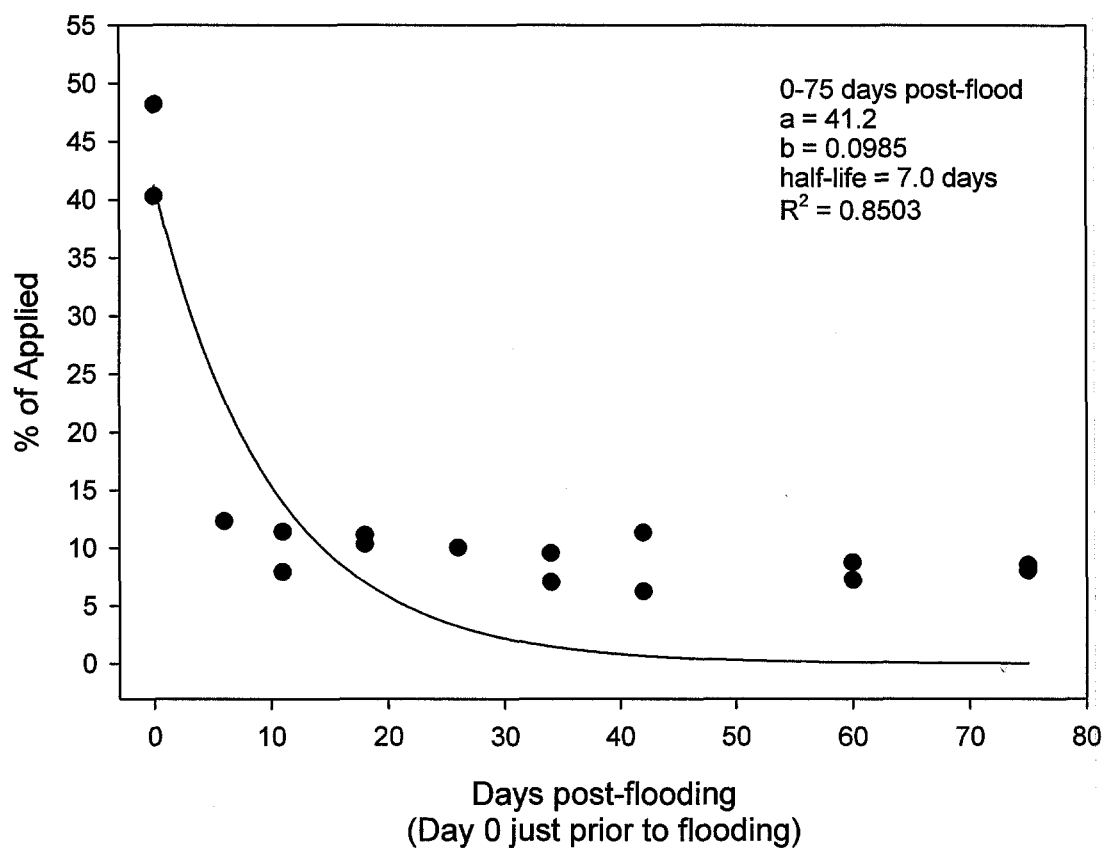
Chemical: Saflufenacil (BAS 800 H)
PC: 118203
MRID: 47611201
Guideline: 835.4200

[Phenyl-U-¹⁴C]saflufenacil in anaerobic Wisconsin
loamy sand soil: soil Rep 2 samples (1/2 model, nonlinear)



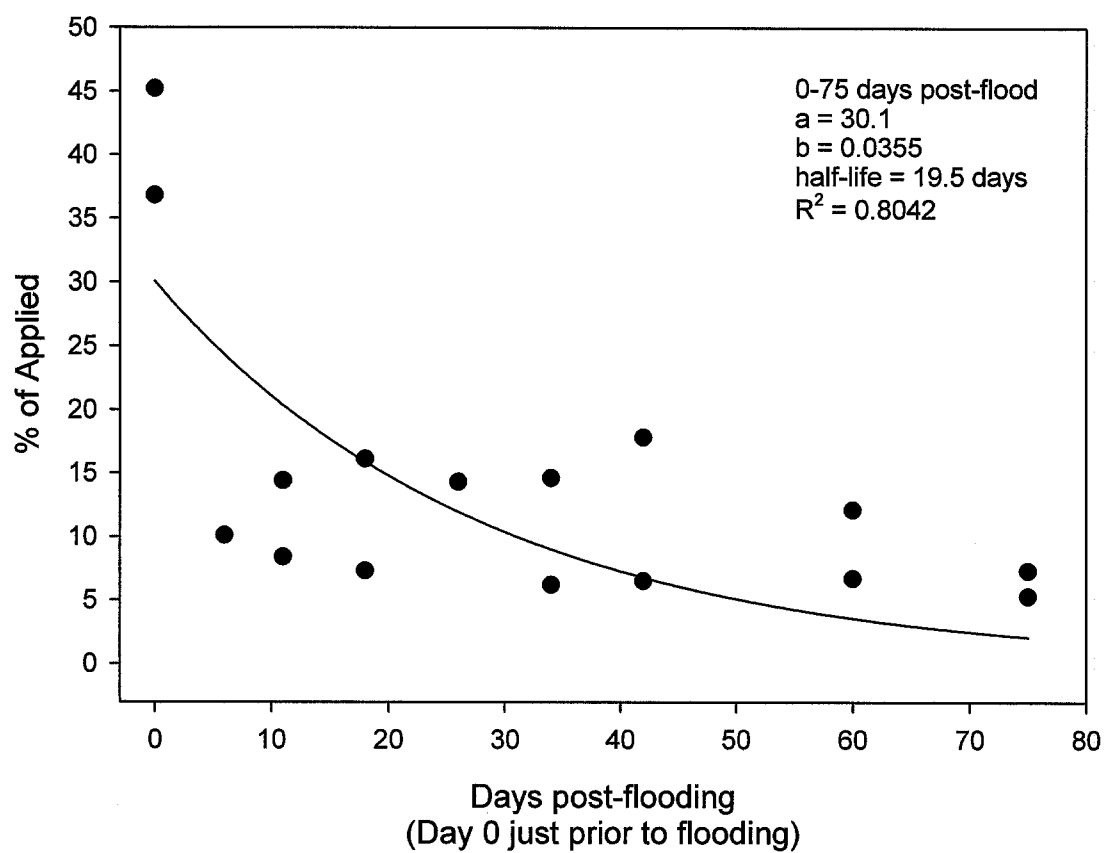
Chemical: Saflufenacil (BAS 800 H)
PC: 118203
MRID: 47611201
Guideline: 835.4200

[Uracil-4-¹⁴C]saflufenacil in anaerobic Wisconsin
loamy sand soil: soil Reps 1 + 2 (1/2 model, nonlinear)



Chemical: Saflufenacil (BAS 800 H)
PC: 118203
MRID: 47611201
Guideline: 835.4200

[Phenyl]-U-¹⁴C]saflufenacil in anaerobic Wisconsin
loamy sand soil: soil Reps 1 + 2 (1/2 model, nonlinear)



Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Phenyl-U-¹⁴C]- and [uracil-4-¹⁴C]-label treated soil.

Nonlinear Regression

Data Source: Data 1 in 118203 47611201 835.4200 Both labels Soil.JNB

Equation: Single, 2 Parameter

R Rsqr Adj Rsqr Standard Error of Estimate

0.9027 0.8148 0.8024 8.0003

	Coefficient	Std. Error	t	P	VIF
a	35.7354	3.6974	9.6649	<0.0001	1.4128
b	0.0612	0.0121	5.0636	<0.0001	1.4128

Analysis of Variance:

	DF	SS	MS
Regression	2	8446.8930	4223.4465
Residual	30	1920.1270	64.0042
Total	32	10367.0200	323.9694

Statistical Tests:

PRESS 2236.0944

Durbin-Watson Statistic 0.6759 Failed

Normality Test Failed (P = 0.0068)

K-S Statistic = 0.2907 Significance Level = 0.0068

Constant Variance Test Passed (P = 0.9529)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	35.7354	1.0646	0.1331	0.1501	0.1476
2	35.7354	9.4646	1.1830	1.3341	1.3524
3	35.7354	12.4646	1.5580	1.7569	1.8238
4	35.7354	4.5646	0.5706	0.6434	0.6370
5	24.7547	-14.6547	-1.8318	-1.9048	-1.9974
6	24.7547	-12.4547	-1.5568	-1.6188	-1.6660
7	18.2301	-9.8301	-1.2287	-1.2742	-1.2881
8	18.2301	-3.8301	-0.4787	-0.4965	-0.4901
9	18.2301	-10.3301	-1.2912	-1.3390	-1.3577
10	18.2301	-6.8301	-0.8537	-0.8853	-0.8821
11	11.8788	-4.5788	-0.5723	-0.5948	-0.5883
12	11.8788	4.2212	0.5276	0.5484	0.5419

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Phenyl-U-¹⁴C]- and [uracil-4-¹⁴C]-label treated soil.

13	11.8788	-0.7788	-0.0974	-0.1012	-0.0995
14	11.8788	-1.5788	-0.1973	-0.2051	-0.2018
15	7.2809	7.0191	0.8774	0.9057	0.9029
16	7.2809	2.7191	0.3399	0.3508	0.3457
17	4.4627	1.7373	0.2172	0.2218	0.2183
18	4.4627	10.1373	1.2671	1.2943	1.3096
19	4.4627	2.5373	0.3172	0.3240	0.3191
20	4.4627	5.0373	0.6296	0.6431	0.6367
21	2.7353	3.7647	0.4706	0.4765	0.4703
22	2.7353	15.0647	1.8830	1.9067	1.9998
23	2.7353	3.4647	0.4331	0.4385	0.4325
24	2.7353	8.5647	1.0706	1.0840	1.0873
25	0.9092	5.7908	0.7238	0.7260	0.7201
26	0.9092	11.1908	1.3988	1.4029	1.4270
27	0.9092	7.7908	0.9738	0.9767	0.9759
28	0.9092	6.2908	0.7863	0.7886	0.7835
29	0.3631	4.9369	0.6171	0.6176	0.6111
30	0.3631	6.9369	0.8671	0.8677	0.8641
31	0.3631	8.1369	1.0171	1.0178	1.0185
32	0.3631	7.6369	0.9546	0.9553	0.9539

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	0.0031	0.2136	0.0769
2	0.2417	0.2136	0.7048
3	0.4192	0.2136	0.9505
4	0.0562	0.2136	0.3320
5	0.1475	0.0752	-0.5695
6	0.1065	0.0752	-0.4750
7	0.0612	0.0701	-0.3537
8	0.0093	0.0701	-0.1346
9	0.0676	0.0701	-0.3728
10	0.0296	0.0701	-0.2422
11	0.0142	0.0743	-0.1666
12	0.0121	0.0743	0.1535
13	0.0004	0.0743	-0.0282
14	0.0017	0.0743	-0.0572
15	0.0269	0.0615	0.2312
16	0.0040	0.0615	0.0885
17	0.0011	0.0416	0.0454
18	0.0363	0.0416	0.2727
19	0.0023	0.0416	0.0664
20	0.0090	0.0416	0.1326
21	0.0029	0.0247	0.0749
22	0.0461	0.0247	0.3184
23	0.0024	0.0247	0.0689
24	0.0149	0.0247	0.1731
25	0.0016	0.0059	0.0554
26	0.0058	0.0059	0.1098
27	0.0028	0.0059	0.0751

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Phenyl-U-¹⁴C]- and [uracil-4-¹⁴C]-label treated soil.

28	0.0018	0.0059	0.0603
29	0.0003	0.0015	0.0237
30	0.0006	0.0015	0.0336
31	0.0008	0.0015	0.0395
32	0.0007	0.0015	0.0370

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	35.7354	28.1843	43.2866	17.7362	53.7347
2	35.7354	28.1843	43.2866	17.7362	53.7347
3	35.7354	28.1843	43.2866	17.7362	53.7347
4	35.7354	28.1843	43.2866	17.7362	53.7347
5	24.7547	20.2749	29.2345	7.8129	41.6964
6	24.7547	20.2749	29.2345	7.8129	41.6964
7	18.2301	13.9034	22.5568	1.3282	35.1320
8	18.2301	13.9034	22.5568	1.3282	35.1320
9	18.2301	13.9034	22.5568	1.3282	35.1320
10	18.2301	13.9034	22.5568	1.3282	35.1320
11	11.8788	7.4263	16.3314	-5.0557	28.8134
12	11.8788	7.4263	16.3314	-5.0557	28.8134
13	11.8788	7.4263	16.3314	-5.0557	28.8134
14	11.8788	7.4263	16.3314	-5.0557	28.8134
15	7.2809	3.2285	11.3333	-9.5529	24.1147
16	7.2809	3.2285	11.3333	-9.5529	24.1147
17	4.4627	1.1320	7.7933	-12.2121	21.1374
18	4.4627	1.1320	7.7933	-12.2121	21.1374
19	4.4627	1.1320	7.7933	-12.2121	21.1374
20	4.4627	1.1320	7.7933	-12.2121	21.1374
21	2.7353	0.1661	5.3045	-13.8042	19.2748
22	2.7353	0.1661	5.3045	-13.8042	19.2748
23	2.7353	0.1661	5.3045	-13.8042	19.2748
24	2.7353	0.1661	5.3045	-13.8042	19.2748
25	0.9092	-0.3437	2.1622	-15.4774	17.2959
26	0.9092	-0.3437	2.1622	-15.4774	17.2959
27	0.9092	-0.3437	2.1622	-15.4774	17.2959
28	0.9092	-0.3437	2.1622	-15.4774	17.2959
29	0.3631	-0.2708	0.9971	-15.9879	16.7142
30	0.3631	-0.2708	0.9971	-15.9879	16.7142
31	0.3631	-0.2708	0.9971	-15.9879	16.7142
32	0.3631	-0.2708	0.9971	-15.9879	16.7142

Fit Equation Description:

[Variables]

x = col(1)

y = col(2)

reciprocal_y = 1/abs(y)

reciprocal_ysquare = 1/y^2

'Automatic Initial Parameter Estimate Functions

F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y))),1,0,1), -306), 0)

assign(q)=if(mean(q)>=0,1,-1)

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Phenyl-U-¹⁴C]- and [uracil-4-¹⁴C]-label treated soil.

[Parameters]

**a = if(F(0)[1]< 307, if(F(0)[1]>-307, assign(y)*10^F(0)[1], assign(y)*10^(-307)), assign(y)*10^307) "Auto
{{previous: 35.7354}}**

b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.061188}}

[Equation]

f = a*exp(-b*x)

fit f to y

"fit f to y with weight reciprocal_y

"fit f to y with weight reciprocal_ysquare

[Constraints]

b>0

[Options]

tolerance=1e-10

stepsize=1

iterations=200

Number of Iterations Performed = 46

Chemical: Saflufenacil (BAS 800 H)
 PC: 118203
 MRID 47611201
 Guideline: 835.4200
 Wisconsin loamy sand soil: soil.
 [Phenyl-U-¹⁴C]-label: Replicate 1 samples.
 Nonlinear Regression

Data Source: Data 1 in 118203 47611201 835.4200 PH Soil Rep 1.JNB
 Equation: Single, 2 Parameter

R Rsqr Adj Rsqr Standard Error of Estimate

0.9414 0.8863 0.8483 5.7329

	Coefficient	Std. Error	t	P	VIF
a	35.6361	5.6665	6.2890	0.0008	1.1821
b	0.1489	0.0501	2.9706	0.0249	1.1821

Analysis of Variance:

	DF	SS	MS
Regression	2	1536.5739	768.2869
Residual	6	197.1961	32.8660
Total	8	1733.7700	216.7212

Statistical Tests:

PRESS 2821.1697

Durbin-Watson Statistic 0.4173 Failed

Normality Test Failed (P = 0.0154)

K-S Statistic = 0.5220 Significance Level = 0.0154

Constant Variance Test Failed (P = 0.0053)

Power of performed test with alpha = 0.0500: 0.9746

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	35.6361	1.1639	0.2030	1.3375	1.4573
2	14.5827	-4.4827	-0.7819	-1.1126	-1.1401
3	6.9257	1.4743	0.2572	0.3267	0.3009
4	2.4420	4.8580	0.8474	0.9095	0.8942
5	0.2254	5.9746	1.0422	1.0444	1.0540
6	0.0685	6.4315	1.1219	1.1222	1.1525
7	0.0047	6.6953	1.1679	1.1679	1.2129
8	0.0005	5.2995	0.9244	0.9244	0.9112

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFBETTS
1	37.9222<	0.9770	9.4895<

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Phenyl-U-¹⁴C]-label: Replicate 1 samples.

2	0.6342	0.5061	-1.1540
3	0.0327	0.3803	0.2357
4	0.0628	0.1319	0.3485
5	0.0023	0.0042	0.0685
6	0.0004	0.0006	0.0282
7	3.9734E-006	5.8264E-006	0.0029
8	4.4972E-008	1.0526E-007	0.0003

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	35.6361	21.7708	49.5014	15.9123	55.3599
2	14.5827	4.6033	24.5622	-2.6327	31.7982
3	6.9257	-1.7246	15.5760	-9.5548	23.4062
4	2.4420	-2.6526	7.5365	-12.4824	17.3663
5	0.2254	-0.6838	1.1346	-13.8319	14.2827
6	0.0685	-0.2747	0.4117	-13.9636	14.1005
7	0.0047	-0.0292	0.0386	-14.0232	14.0326
8	0.0005	-0.0040	0.0051	-14.0274	14.0284

Fit Equation Description:

[Variables]

x = col(1)

y = col(2)

reciprocal_y = 1/abs(y)

reciprocal_ysquare = 1/y^2

'Automatic Initial Parameter Estimate Functions

F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)

assign(q)=if(mean(q)>=0,1,-1)

[Parameters]

a = if(F(0)[1]< 307, if(F(0)[1]>-307, assign(y)*10^F(0)[1], assign(y)*10^(-307)), assign(y)*10^307) "Auto

{previous: 35.6361}}

b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {previous: 0.14892}}

[Equation]

f = a*exp(-b*x)

fit f to y

"fit f to y with weight reciprocal_y

"fit f to y with weight reciprocal_ysquare

[Constraints]

b>0

[Options]

tolerance=1e-10

stepsize=1

iterations=200

Number of Iterations Performed = 15

Chemical: Saflufenacil (BAS 800 H)
 PC: 118203
 MRID 47611201
 Guideline: 835.4200
 Wisconsin loamy sand soil: soil.
 [Uracil-4-¹⁴C]-label: Replicates 1 and 2.
 Nonlinear Regression

Data Source: Data 1 in 118203 47611201 835.4200 UR Soil Both Reps.JNB
 Equation: Single, 2 Parameter

R Rsqr Adj Rsqr Standard Error of Estimate

0.9221 0.8503 0.8290 7.4482

	Coefficient	Std. Error	t	P	VIF
a	41.1821	5.1255	8.0347	<0.0001	1.2322
b	0.0985	0.0249	3.9636	0.0014	1.2322

Analysis of Variance:

	DF	SS	MS
Regression	2	4412.7877	2206.3938
Residual	14	776.6623	55.4759
Total	16	5189.4500	324.3406

Statistical Tests:

PRESS 1020.9352

Durbin-Watson Statistic 0.3773 Failed

Normality Test Failed (P = 0.0013)

K-S Statistic = 0.4618 Significance Level = 0.0013

Constant Variance Test Passed (P = 0.0619)

Power of performed test with alpha = 0.0500: 0.9999

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	41.1821	7.0179	0.9422	1.2986	1.3343
2	41.1821	-0.8821	-0.1184	-0.1632	-0.1574
3	22.8006	-10.5006	-1.4098	-1.5788	-1.6781
4	13.9308	-6.0308	-0.8097	-0.9124	-0.9066
5	13.9308	-2.5308	-0.3398	-0.3829	-0.3709
6	6.9891	4.1109	0.5519	0.5977	0.5835
7	6.9891	3.3109	0.4445	0.4814	0.4678
8	3.1774	6.8226	0.9160	0.9479	0.9442
9	1.4445	5.5555	0.7459	0.7550	0.7428
10	1.4445	8.0555	1.0815	1.0948	1.1032
11	0.6567	5.5433	0.7442	0.7471	0.7348
12	0.6567	10.6433	1.4290	1.4345	1.4967

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Uracil-4-¹⁴C]-label: Replicates 1 and 2.

13	0.1114	8.5886	1.1531	1.1534	1.1683
14	0.1114	7.0886	0.9517	0.9519	0.9485
15	0.0254	8.4746	1.1378	1.1378	1.1509
16	0.0254	7.9746	1.0707	1.0707	1.0768

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	0.7585	0.4736	1.2655
2	0.0120	0.4736	-0.1493
3	0.3167	0.2026	-0.8459
4	0.1123	0.2124	-0.4708
5	0.0198	0.2124	-0.1926
6	0.0309	0.1474	0.2426
7	0.0200	0.1474	0.1945
8	0.0318	0.0661	0.2513
9	0.0070	0.0240	0.1165
10	0.0147	0.0240	0.1731
11	0.0022	0.0077	0.0648
12	0.0080	0.0077	0.1320
13	0.0003	0.0005	0.0252
14	0.0002	0.0005	0.0205
15	2.4810E-005	3.8326E-005	0.0071
16	2.1969E-005	3.8326E-005	0.0067

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	41.1821	30.1890	52.1753	21.7903	60.5740
2	41.1821	30.1890	52.1753	21.7903	60.5740
3	22.8006	15.6096	29.9915	5.2818	40.3193
4	13.9308	6.5679	21.2937	-3.6592	31.5208
5	13.9308	6.5679	21.2937	-3.6592	31.5208
6	6.9891	0.8562	13.1219	-10.1225	24.1007
7	6.9891	0.8562	13.1219	-10.1225	24.1007
8	3.1774	-0.9310	7.2858	-13.3173	19.6720
9	1.4445	-1.0313	3.9203	-14.7211	17.6100
10	1.4445	-1.0313	3.9203	-14.7211	17.6100
11	0.6567	-0.7468	2.0602	-15.3797	16.6931
12	0.6567	-0.7468	2.0602	-15.3797	16.6931
13	0.1114	-0.2332	0.4561	-15.8671	16.0900
14	0.1114	-0.2332	0.4561	-15.8671	16.0900
15	0.0254	-0.0735	0.1243	-15.9497	16.0006
16	0.0254	-0.0735	0.1243	-15.9497	16.0006

Fit Equation Description:

[Variables]

x = col(1)

y = col(2)

reciprocal_y = 1/abs(y)

reciprocal_ysquare = 1/y^2

'Automatic Initial Parameter Estimate Functions

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Uracil-4-¹⁴C]-label: Replicates 1 and 2.

$F(q) = \text{if}(\text{size}(x) > 1, \text{if}(\text{total}(\text{abs}(y)) > 0, \text{ape}(x, \log(\text{abs}(y))), 1, 0, 1), -306), 0)$

$\text{assign}(q) = \text{if}(\text{mean}(q) \geq 0, 1, -1)$

[Parameters]

$a = \text{if}(F(0)[1] < 307, \text{if}(F(0)[1] > -307, \text{assign}(y) * 10^{F(0)[1]}, \text{assign}(y) * 10^{(-307)}), \text{assign}(y) * 10^{307})$ "Auto
{previous: 41.1821}}

$b = \text{if}(x50(x, y) - \min(x) = 0, 1, -\ln(.5)/(x50(x, y) - \min(x)))$ "Auto {previous: 0.0985366}}

[Equation]

$f = a * \exp(-b * x)$

fit f to y

"fit f to y with weight reciprocal_y

"fit f to y with weight reciprocal_ysquare

[Constraints]

$b > 0$

[Options]

tolerance=1e-10

stepsize=1

iterations=200

Number of Iterations Performed = 30

Chemical: Saflufenacil (BAS 800 H)
 PC: 118203
 MRID 47611201
 Guideline: 835.4200
 Wisconsin loamy sand soil: soil.
 [Phenyl-U-¹⁴C]-label: Replicates 1 and 2.
 Nonlinear Regression

Data Source: Data 1 in 118203 47611201 835.4200 PH Both Reps.JNB
 Equation: Single, 2 Parameter

R Rsqr Adj Rsqr Standard Error of Estimate

0.8968 0.8042 0.7762 8.5099

	Coefficient	Std. Error	t	P	VIF
a	30.0769	5.0257	5.9846	<0.0001	1.6053
b	0.0355	0.0115	3.0743	0.0082	1.6053

Analysis of Variance:

	DF	SS	MS
Regression	2	4163.7061	2081.8530
Residual	14	1013.8639	72.4189
Total	16	5177.5700	323.5981

Statistical Tests:

PRESS 1580.8747

Durbin-Watson Statistic 1.4242 Failed

Normality Test Passed (P = 0.6613)

K-S Statistic = 0.1759 Significance Level = 0.6613

Constant Variance Test Passed (P = 0.0675)

Power of performed test with alpha = 0.0500: 0.9995

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	30.0769	6.7231	0.7900	0.9790	0.9774
2	30.0769	15.1231	1.7771	2.2022<	2.6248<
3	24.3075	-14.2075	-1.6695	-1.8119	-1.9956
4	20.3546	-11.9546	-1.4048	-1.4832	-1.5567
5	20.3546	-5.9546	-0.6997	-0.7388	-0.7262
6	15.8765	-8.5765	-1.0078	-1.0618	-1.0670
7	15.8765	0.2235	0.0263	0.0277	0.0267
8	11.9517	2.3483	0.2760	0.2927	0.2829
9	8.9971	-2.7971	-0.3287	-0.3491	-0.3379
10	8.9971	5.6029	0.6584	0.6992	0.6859
11	6.7730	-0.2730	-0.0321	-0.0339	-0.0327
12	6.7730	11.0270	1.2958	1.3686	1.4170

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Phenyl-U-¹⁴C]-label: Replicates 1 and 2.

13	3.5752	3.1248	0.3672	0.3797	0.3677
14	3.5752	8.5248	1.0017	1.0357	1.0386
15	2.0993	3.2007	0.3761	0.3832	0.3712
16	2.0993	5.2007	0.6111	0.6226	0.6084

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	0.2566	0.3488	0.7153
2	1.2986	0.3488	1.9209
3	0.2919	0.1510	-0.8415
4	0.1262	0.1029	-0.5273
5	0.0313	0.1029	-0.2460
6	0.0620	0.0991	-0.3538
7	4.2115E-005	0.0991	0.0088
8	0.0054	0.1113	0.1001
9	0.0078	0.1134	-0.1208
10	0.0313	0.1134	0.2453
11	6.6347E-005	0.1036	-0.0111
12	0.1083	0.1036	0.4818
13	0.0050	0.0645	0.0966
14	0.0370	0.0645	0.2728
15	0.0028	0.0365	0.0723
16	0.0073	0.0365	0.1185

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	30.0769	19.2979	40.8560	8.8797	51.2742
2	30.0769	19.2979	40.8560	8.8797	51.2742
3	24.3075	17.2158	31.3992	4.7262	43.8888
4	20.3546	14.4994	26.2098	1.1864	39.5228
5	20.3546	14.4994	26.2098	1.1864	39.5228
6	15.8765	10.1314	21.6215	-3.2583	35.0113
7	15.8765	10.1314	21.6215	-3.2583	35.0113
8	11.9517	5.8620	18.0413	-7.2894	31.1927
9	8.9971	2.8502	15.1441	-10.2621	28.2564
10	8.9971	2.8502	15.1441	-10.2621	28.2564
11	6.7730	0.8979	12.6481	-12.4013	25.9472
12	6.7730	0.8979	12.6481	-12.4013	25.9472
13	3.5752	-1.0618	8.2122	-15.2566	22.4070
14	3.5752	-1.0618	8.2122	-15.2566	22.4070
15	2.0993	-1.3886	5.5872	-16.4830	20.6815
16	2.0993	-1.3886	5.5872	-16.4830	20.6815

Fit Equation Description:

[Variables]

x = col(1)

y = col(2)

reciprocal_y = 1/abs(y)

reciprocal_ysquare = 1/y^2

'Automatic Initial Parameter Estimate Functions

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Phenyl-U-¹⁴C]-label: Replicates 1 and 2.

$F(q) = \text{if}(\text{size}(x) > 1, \text{if}(\text{total}(\text{abs}(y)) > 0, \text{ape}(x, \log(\text{abs}(y))), 1, 0, 1), -306), 0)$

$\text{assign}(q) = \text{if}(\text{mean}(q) \geq 0, 1, -1)$

[Parameters]

$a = \text{if}(F(0)[1] < 307, \text{if}(F(0)[1] > -307, \text{assign}(y) * 10^{F(0)[1]}, \text{assign}(y) * 10^{(-307)}), \text{assign}(y) * 10^{307})$ "Auto
{ {previous: 30.0769} }

$b = \text{if}(x50(x, y) - \min(x) = 0, 1, -\ln(.5)/(x50(x, y) - \min(x)))$ "Auto { {previous: 0.0354956} }

[Equation]

$f = a * \exp(-b * x)$

fit f to y

"fit f to y with weight reciprocal_y

"fit f to y with weight reciprocal_ysquare

[Constraints]

$b > 0$

[Options]

tolerance=1e-10

stepsize=1

iterations=200

Number of Iterations Performed = 23

Chemical: Saflufenacil (BAS 800 H)
 PC: 118203
 MRID 47611201
 Guideline: 835.4200
 Wisconsin loamy sand soil: soil.
 [Phenyl-U-¹⁴C]-label: Replicate 2 samples.
 Nonlinear Regression

Data Source: Data 1 in 118203 47611201 835.4200 PH Soil Rep 2.JNB
 Equation: Single, 2 Parameter

R Rsqr Adj Rsqr Standard Error of Estimate

0.9472 0.8973 0.8630 7.6788

	Coefficient	Std. Error	t	P	VIF
a	35.8015	6.5907	5.4321	0.0016	1.7760
b	0.0283	0.0097	2.9214	0.0266	1.7760

Analysis of Variance:

	DF	SS	MS
Regression	2	3090.0173	1545.0086
Residual	6	353.7827	58.9638
Total	8	3443.8000	430.4750

Statistical Tests:

PRESS 1693.5221

Durbin-Watson Statistic 1.5708 Passed

Normality Test Passed (P = 0.9395)

K-S Statistic = 0.1782 Significance Level = 0.9395

Constant Variance Test Passed (P = 0.2327)

Power of performed test with alpha = 0.0500: 0.9810

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	35.8015	9.3985	1.2240	2.3852<	9.5661<
2	26.2103	-11.8103	-1.5380	-1.7470	-2.2752<
3	21.4926	-5.3926	-0.7023	-0.7715	-0.7421
4	17.1315	-2.8315	-0.3687	-0.4072	-0.3769
5	13.6553	0.9447	0.1230	0.1373	0.1256
6	10.8844	6.9156	0.9006	1.0085	1.0103
7	6.5342	5.5658	0.7248	0.7944	0.7666
8	4.2709	3.0291	0.3945	0.4204	0.3896

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	7.9581<	0.7367	16.0004<

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID 47611201

Guideline: 835.4200

Wisconsin loamy sand soil: soil.

[Phenyl-U-¹⁴C]-label: Replicate 2 samples.

2	0.4428	0.2249	-1.2256
3	0.0616	0.1715	-0.3376
4	0.0182	0.1799	-0.1765
5	0.0023	0.1975	0.0623
6	0.1292	0.2026	0.5092
7	0.0634	0.1674	0.3437
8	0.0120	0.1196	0.1435

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	35.8015	19.6746	51.9284	11.0403	60.5627
2	26.2103	17.2992	35.1213	5.4150	47.0056
3	21.4926	13.7117	29.2735	1.1559	41.8293
4	17.1315	9.1620	25.1009	-3.2781	37.5410
5	13.6553	5.3052	22.0053	-6.9059	34.2164
6	10.8844	2.4281	19.3407	-9.7201	31.4890
7	6.5342	-1.1536	14.2220	-13.7670	26.8355
8	4.2709	-2.2258	10.7675	-15.6099	24.1516

Fit Equation Description:

[Variables]

x = col(1)

y = col(2)

reciprocal_y = 1/abs(y)

reciprocal_ysquare = 1/y^2

'Automatic Initial Parameter Estimate Functions

F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y))),1,0,1), -306), 0)

assign(q)=if(mean(q)>=0,1,-1)

[Parameters]

a = if(F(0)[1]< 307, if(F(0)[1]>-307, assign(y)*10^F(0)[1], assign(y)*10^(-307)), assign(y)*10^307) "Auto

{{previous: 35.8015}}

b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.028349}}

[Equation]

f = a*exp(-b*x)

fit f to y

"fit f to y with weight reciprocal_y

"fit f to y with weight reciprocal_ysquare

[Constraints]

b>0

[Options]

tolerance=1e-10

stepsize=1

iterations=200

Number of Iterations Performed = 14

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Half-life determination.

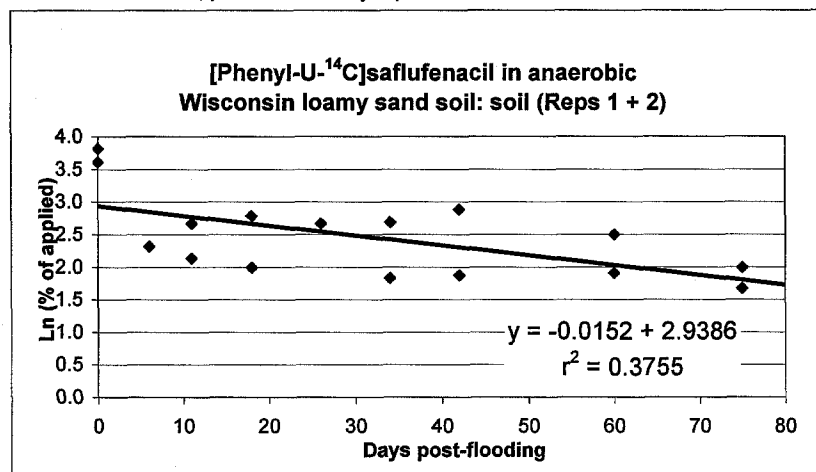
[Phenyl- ^{14}C]-label treated soil: Replicates 1 and 2.

Half-life (days) 45.7 (0- to 75-day post-flood data)

Days Post-flooding	Saflufenacil		Rep
	(% of Applied)	Ln (% applied)	
0	36.8	3.605497845	1
0	45.2	3.811097087	2
6	10.1	2.312535424	1
11	8.4	2.128231706	1
11	14.4	2.667228207	2
18	7.3	1.987874348	1
18	16.1	2.778819272	2
26	14.3	2.660259537	2
34	6.2	1.824549292	1
34	14.6	2.681021529	2
42	6.5	1.871802177	1
42	17.8	2.879198457	2
60	6.7	1.902107526	1
60	12.1	2.493205453	2
75	5.3	1.667706821	1
75	7.3	1.987874348	2

Day 0 just prior to flooding.

Results from Table 6, p. 45 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.61280526
R Square	0.375530287
Adjusted R Square	0.330925307
Standard Error	0.509236129
Observations	16

ANOVA

	df	SS	MS	F	Sig F
Regression	1	2.183232762	2.183	8.41902161	0.0116063
Residual	14	3.630500085	0.259		
Total	15	5.813732848			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	2.938591668	0.210086153	13.99	1.27826E-09	2.4880017	3.3891817	2.48800168	3.38918165
X Variable 1	-0.015153238	0.005222454	-2.902	0.011606331	-0.026354	-0.0039522	-0.0263543	-0.0039522

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Half-life determination.

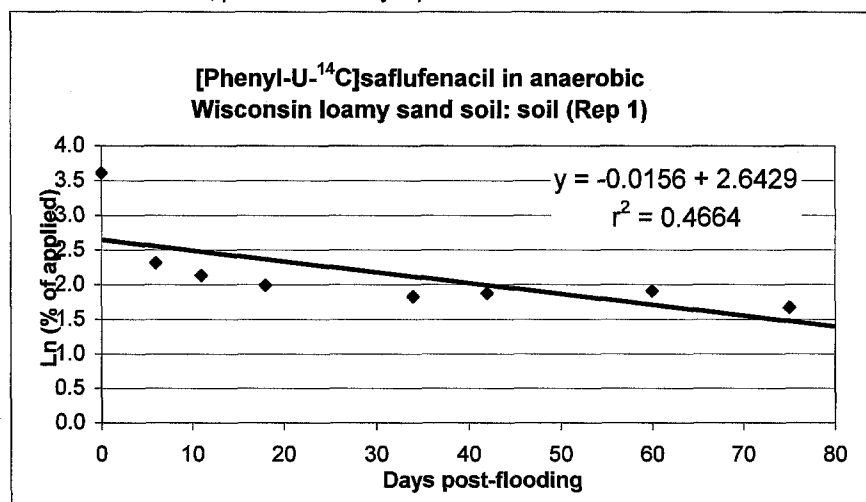
[Phenyl- ^{14}C]-label treated soil: Replicate 1 samples.

Half-life (days) 44.4 (0- to 75-day post-flood data)

Days Post-flooding	Saflufenacil		Rep
	(% of Applied)	Ln (% applied)	
0	36.8	3.605497845	1
6	10.1	2.312535424	1
11	8.4	2.128231706	1
18	7.3	1.987874348	1
34	6.2	1.824549292	1
42	6.5	1.871802177	1
60	6.7	1.902107526	1
75	5.3	1.667706821	1

Day 0 just prior to flooding.

Results from Table 6, p. 45 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.682950099
R Square	0.466420837
Adjusted R Square	0.377490977
Standard Error	0.485247493
Observations	8

ANOVA

	df	SS	MS	F	Sig F
Regression	1	1.234971494	1.235	5.244816927	0.0619307
Residual	6	1.412790774	0.235		
Total	7	2.647762268			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	2.642861787	0.27096399	9.754	6.67648E-05	1.9798368	3.3058868	1.97983679	3.30588678
X Variable 1	-0.015620281	0.006820617	-2.29	0.061930749	-0.03231	0.0010692	-0.0323097	0.00106917

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Half-life determination.

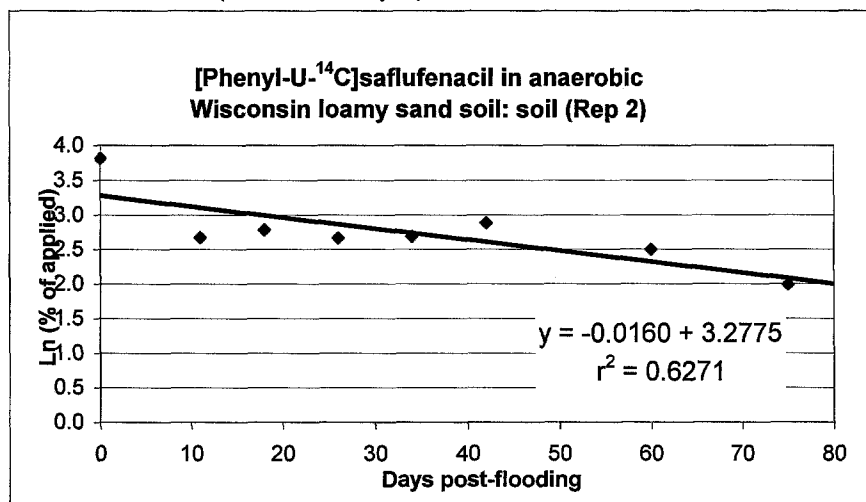
[Phenyl- ^{14}C]-label treated soil: Replicate 2 samples.

Half-life (days) 43.3 (0- to 75-day post-flood data)

Days Post-flooding	Saflufenacil		Rep
	(% of Applied)	Ln (% applied)	
0	45.2	3.811097087	2
11	14.4	2.667228207	2
18	16.1	2.778819272	2
26	14.3	2.660259537	2
34	14.6	2.681021529	2
42	17.8	2.879198457	2
60	12.1	2.493205453	2
75	7.3	1.987874348	2

Day 0 just prior to flooding.

Results from Table 6, p. 45 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.791918281
R Square	0.627134564
Adjusted R Square	0.564990324
Standard Error	0.335352161
Observations	8

ANOVA

	df	SS	MS	F	Sig F
Regression	1	1.134911715	1.135	10.09159609	0.019155
Residual	6	0.674766432	0.112		
Total	7	1.809678147			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	3.277544337	0.205372031	15.96	3.84333E-06	2.7750171	3.7800716	2.77501708	3.78007159
X Variable 1	-0.016021244	0.005043317	-3.177	0.019154998	-0.028362	-0.0036807	-0.0283618	-0.00368069

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Half-life determination.

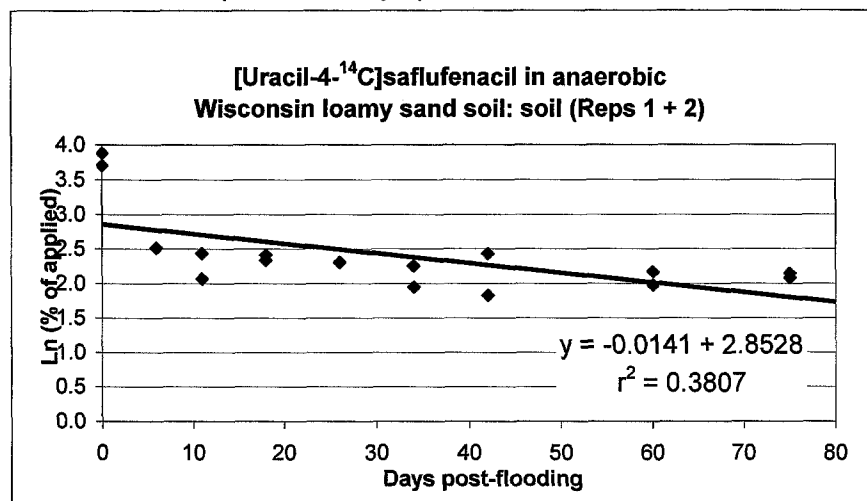
[Uracil-4- ^{14}C]-label treated soil: Replicates 1 and 2.

Half-life (days) 49.2 (0- to 75-day post-flood data)

Days Post-flooding	Saflufenacil		Rep
	(% of Applied)	Ln (% applied)	
0	48.2	3.875359021	1
0	40.3	3.696351469	2
6	12.3	2.509599262	1
11	7.9	2.066862759	1
11	11.4	2.433613355	2
18	11.1	2.406945108	1
18	10.3	2.332143895	2
26	10.0	2.302585093	2
34	7.0	1.945910149	1
34	9.5	2.251291799	2
42	6.2	1.824549292	1
42	11.3	2.424802726	2
60	8.7	2.163323026	1
60	7.2	1.974081026	2
75	8.5	2.140066163	1
75	8.0	2.079441542	2

Day 0 just prior to flooding.

Results from Table 7, p. 48 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.617044662
R Square	0.380744115
Adjusted R Square	0.336511552
Standard Error	0.46854792
Observations	16

ANOVA

	df	SS	MS	F	Sig F
Regression	1	1.889727237	1.89	8.607778707	0.0108872
Residual	14	3.073520151	0.22		
Total	15	4.963247388			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	2.852816226	0.19330017	14.76	6.30755E-10	2.4382286	3.2674039	2.4382286	3.26740386
X Variable 1	-0.014097918	0.004805177	-2.934	0.010887249	-0.024404	-0.0037918	-0.024404	-0.00379184

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

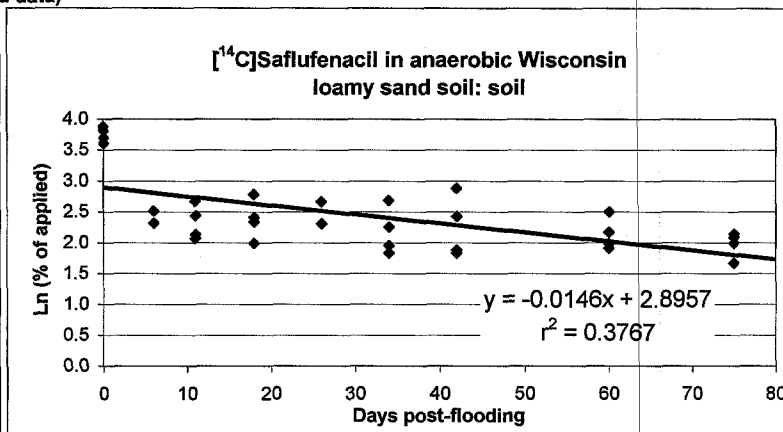
Anaerobic metabolism of [14 C]saflufenacil in Wisconsin loamy sand soil.

Half-life determination.

[Phenyl- 14 C]- and [uracil- 14 C]-label treated soil.

Half-life (days) 47.4 (0- to 75-day post-flood data)

Days Post-flooding	Saflufenacil		
	(% of Applied)	Ln (% applied)	Label
0	36.8	3.605497845	PH
0	45.2	3.811097087	PH
0	48.2	3.875359021	UR
0	40.3	3.696351469	UR
6	10.1	2.312535424	PH
6	12.3	2.509599262	UR
11	8.4	2.128231706	PH
11	14.4	2.667228207	PH
11	7.9	2.066862759	UR
11	11.4	2.433613355	UR
18	7.3	1.987874348	PH
18	16.1	2.778819272	PH
18	11.1	2.406945108	UR
18	10.3	2.332143895	UR
26	14.3	2.660259537	PH
26	10.0	2.302585093	UR
34	6.2	1.824549292	PH
34	14.6	2.681021529	PH
34	7.0	1.945910149	UR
34	9.5	2.251291799	UR
42	6.5	1.871802177	PH
42	17.8	2.879198457	PH
42	6.2	1.824549292	UR
42	11.3	2.424802726	UR
60	6.7	1.902107526	PH
60	12.1	2.493205453	PH
60	8.7	2.163323026	UR
60	7.2	1.974081026	UR
75	5.3	1.667706821	PH
75	7.3	1.987874348	PH
75	8.5	2.140066163	UR
75	8.0	2.079441542	UR



Day 0 just prior to flooding.

Results from Table 6, p. 45; Table 7, p. 48 of the study report.

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.613745829
R Square	0.376683943
Adjusted R Square	0.355906741
Standard Error	0.473671866
Observations	32

ANOVA

	df	SS	MS	F	Sig F
Regression	1	4.06766547	4.07	18.12967622	0.0001871
Residual	30	6.7309511	0.22		
Total	31	10.79861657			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	2.895703947	0.138178608	21	1.82027E-19	2.6135056	3.1779023	2.61350558	3.177902311
X Variable 1	-0.014625578	0.003434931	-4.26	0.000187142	-0.021641	-0.0076105	-0.02164064	-0.00761051

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Nonlinear half-lives (exponential decay/single compartment, 2 parameter):

[Phenyl-U- ^{14}C]-label (both Replicates):

Phase	water	soil	system
Half-life (days)	ND	19.5	ND
r squared		0.8042	

[Phenyl-U- ^{14}C]-label (Replicate 1 samples):

Phase	water	soil	system
Half-life (days)	ND	4.7	ND
r squared		0.8863	

[Phenyl-U- ^{14}C]-label (Replicate 2 samples):

Phase	water	soil	system
Half-life (days)	ND	24.5	ND
r squared		0.8973	

[Uracil-4- ^{14}C]-label (both Replicates):

Phase	water	soil	system
Half-life (days)	ND	7.0	ND
r squared		0.8503	

Both labels (all Replicates):

Phase	water	soil	system
Half-life (days)	ND	11.3	ND
r squared		0.8148	

ND = Not determined due to insufficient dissipation.

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Determination of means/standard deviations of treated system parameters (pH, O_2 and redox potentials).

Day ¹	[Phenyl- ^{14}C]-label			[Uracyl- ^{14}C]-label			Labels combined					
	Water	Interface	Soil	Water	Interface	Soil	Water		Interface		Soil	
	pH ²	O_2 (mg/L)	Redox (mV)	pH ²	O_2 (mg/L)	Redox (mV)	pH ²		O_2 (mg/L)		Redox (mV)	
							mean	s.d.	mean	s.d.	mean	s.d.
23	5.0	0.25	-213	5.0		-11	5.0	0.0	0.25	0.00	-112	101
28	5.0	0.25	113	5.0	0.22	-55						
	5.0	0.24	102	5.0	0.25	97	5.0	0.0	0.24	0.01	64	69
35	5.0	0.15	25	5.0		49						
	5.0	0.14	28	5.0	0.15	18	5.0	0.0	0.15	0.00	30	12
43	5.5	0.13	-3	5.5	0.13	-1	5.5	0.0	0.13	0.00	-2	1
51	5.5	0.13	-73	5.5	0.13	-218						
	5.5	0.11	-224	5.5	0.13	-213	5.5	0.0	0.13	0.01	-182	63
57	5.5	0.14	-6	5.0	0.13	-30						
	5.5	0.13	-34	5.5	0.14	-15	5.4	0.2	0.14	0.01	-21	11
77	5.0	0.15	-21	5.5	0.14	-36						
	5.5	0.15	-18	5.0	0.14	-31	5.3	0.3	0.15	0.00	-27	7
92	5.5	0.14	-30	5.5	0.14	-36						
	6.0	0.15	-85	5.5	0.14	-27	5.6	0.2	0.14	0.00	-45	24
Mean	5.3	0.16	-31	5.3	0.15	-36	5.3		0.16		-34	
std.dev.	0.3	0.05	93	0.3	0.04	82	0.3		0.04		88	
max	6.0	0.25	113	5.5	0.25	97	6.0		0.25		113	
min	5.0	0.11	-224	5.0	0.13	-218	5.0		0.11		-224	
n =	14	14	14	14	12	14	28		26		28	

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

2 Determined using pH paper (p. 24).

Blank cell indicates no result provided.

Parameters measured in untreated water-soil systems at 23 days, but determined in treated systems at all remaining intervals.

Results from Table 2, p. 41 of the study report.

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)
 PC: 118203
 MRID: 47611201
 Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.
 [Phenyl-U-¹⁴C]-label.

Day ¹	Water			Soil						Volatiles						Material Balance			Study Reported		
	Water			Extractable			Nonextractable			CO ₂			Volatile Organics			Material Balance			Material Balance		
	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0				99.5	99.5	0.0	0.5	0.5	0.0							100.0	100.0	0.0	100.0	100.0	0.0
14				99.5	99.5	0.0	0.5	0.5	0.0							100.0	100.0	0.0	100.0	100.0	0.0
17				93.8	92.2	1.6	5.8	6.3	0.5	0.1	0.1	0.1				99.7	98.5	1.2	99.6	98.5	1.2
23				90.5	89.4	0.7	6.3	6.9	0.6	0.1	0.1	0.0				97.3	96.4	0.1	97.3	96.2	0.1
28				88.7	89.4	0.7	7.5	4.8		0.1	0.1	0.0				96.5	96.4	0.1	96.3	96.2	0.1
35				26.8			4.8			0.1	0.1	0.0				96.3			96.1		
43				25.0			5.0			0.1	0.1	0.0				95.6			95.5		
51				63.7	64.5	0.7	24.5	24.8	0.3							95.2	93.9	1.3	95.2	94.0	1.3
59				24.0	25.3	1.3	5.3	5.0	0.3	0.1	0.1	0.0	0.0	0.0	0.0	100.3	103.0	2.7	100.2	102.9	2.7
77				26.6			4.7			0.1	0.1	0.0	0.0	0.0	0.0	105.6			105.5		
92				23.4			5.2			0.1	0.1	0.0	0.0	0.0	0.0	99.8			99.6		
				21.9			4.4			0.1	0.1	0.0	0.0	0.0	0.0	98.2	95.8	2.4	98.0	95.6	2.4
				22.6	22.3	0.4	3.8	4.1	0.3	0.1	0.1	0.0	0.0	0.0	0.0	93.3	98.9	0.1	93.2	98.8	0.1
				22.6	23.5	0.9	5.2	4.4	0.9	0.1	0.1	0.0	0.0	0.0	0.0	98.7	99.0	0.5	98.7	99.3	0.5
				24.4	23.5	0.9	3.5	5.0	0.8	0.1	0.1	0.0	0.0	0.0	0.0	98.4	99.0	0.5	96.7	98.0	1.3
				21.0	21.1	0.1	5.8	5.2	0.8	0.1	0.1	0.0	0.0	0.0	0.0	99.5	98.7	0.0	99.3	98.6	0.0
				21.1	21.1	0.1	4.2	5.2	0.3	0.1	0.1	0.0	0.0	0.0	0.0	98.7	98.7	0.0	98.6	98.6	0.0
				20.0	19.9	0.1	5.5	5.2	0.3	0.1	0.1	0.0	0.0	0.0	0.0	98.6	98.7	0.0	98.5	98.6	0.0
				19.8			4.9			0.1	0.1	0.0	0.0	0.0	0.0	98.6			98.5		
Overall																98.2	2.8		98.0	2.8	
maximum																105.6			105.5		
minimum																92.6			92.7		
n =																20			20		

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 4, p. 43 of the study report.

Shaded block indicates result does not agree (>0.1%) with that reported by the study authors (Reviewer's Comment No. 1).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.

[Uracil-4-¹⁴C]-label.

Day ¹	Water			Soil						Volatiles						Material Balance			Study Reported Material Balance		
				Extractable			Nonextractable			CO ₂			Volatile Organics								
	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0				100.4			0.3									100.7			100.6		
				99.7	100.1	0.3	0.3	0.3	0.0							100.0	100.4	0.3	100.0	100.3	0.3
14				91.8			4.4			0.1						96.3			96.3		
				93.6	92.7	0.9	5.4	4.9	0.5	0.1	0.1	0.0				99.1	97.7	1.4	99.1	97.7	1.4
17				94.7			4.8			0.2						99.7			99.5		
				91.4	93.1	1.6	5.7	5.3	0.5	0.1	0.2	0.1				97.2	98.5	1.3	97.1	98.3	1.2
23	69.7			25.1			3.5			0.2						98.5			98.3		
										0.1	0.2	0.1									
28	74.6			19.4			3.5									97.5			97.6		
	72.2	73.4	1.2	23.0	21.2	1.8	3.5	3.5	0.0							98.7	98.1	0.6	98.7	98.2	0.5
35	73.0			21.9			3.4			0.2			0.0			98.5			98.3		
	72.5	72.8	0.3	23.2	22.6	0.7	3.9	3.7	0.2	0.2	0.2	0.0	0.0	0.0	0.0	99.8	99.2	0.7	99.7	99.0	0.7
43										0.3			0.0								
	74.9			21.2			3.4			0.2	0.3	0.1	0.0	0.0	0.0	99.7			99.5		
51	73.2			18.8			3.6			0.3			0.1			96.0			95.6		
	73.5	73.4	0.1	23.2	21.0	2.2	3.9	3.8	0.2	0.2	0.3	0.1	0.1	0.1	0.0	100.9	98.5	2.5	100.6	98.1	2.5
59	77.4			18.3			3.3			0.5			0.2			99.7			99.0		
	69.0	73.2	4.2	25.5	21.9	3.6	4.5	3.9	0.6	0.3	0.4	0.1	0.1	0.2	0.1	99.4	99.6	0.2	98.9	99.0	0.0
77	71.5			21.4			3.8			0.5			0.3			97.5			96.7		
	74.6	73.1	1.6	21.1	21.3	0.1	4.1	4.0	0.2	0.3	0.4	0.1	0.1	0.2	0.1	100.2	98.9	1.3	99.7	98.2	1.5
92	74.0			20.6			3.7			0.5			0.3			99.1			98.3		
	75.8	74.9	0.9	19.5	20.1	0.6	3.8	3.8	0.0	0.4	0.5	0.1	0.2	0.3	0.1	99.7	99.4	0.3	99.0	98.7	0.3
Overall																98.9	1.3		98.6	1.3	
maximum																100.9			100.6		
minimum																96.0			95.6		
n =																20			20		

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 5, p. 44 of the study report.

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 5, p. 44 of the study report.

Shaded block indicates result does not agree (>0.1%) with that reported by the study authors (Reviewer's Comment No. 1).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Labels combined				
Overall	98.5	2.2	98.3	2.2
maximum	105.6		105.5	
minimum	92.6		92.7	
n =	40		40	

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

Determination of means/standard deviations for applied radioactivity in water layers and soil for labels combined.

Day ¹	Label	Water			Soil					
		% AR	Mean	s.d.	Extractable			Nonextractable		
					% AR	Mean	s.d.	% AR	Mean	s.d.
0	PH				99.5			0.5		
	PH				99.5			0.5		
	UR				100.4			0.3		
	UR				99.7	99.8	0.4	0.3	0.4	0.1
14	PH				93.8			5.8		
	PH				90.5			6.8		
	UR				91.8			4.4		
	UR				93.6	92.4	1.4	5.4	5.6	0.9
17	PH				90.1			6.3		
	PH				88.7			7.5		
	UR				94.7			4.8		
	UR				91.4	91.2	2.2	5.7	6.1	1.0
23	PH	63.9			26.8			4.8		
	UR	69.7	66.8	2.9	25.1	26.0	0.8	3.5	4.2	0.6
28	PH	65.2			25.0			5.0		
	PH	63.7			24.5			4.4		
	UR	74.6			19.4			3.5		
	UR	72.2	68.9	4.6	23.0	23.0	2.2	3.5	4.1	0.6
35	PH	70.9			24.0			5.3		
	PH	74.2			26.6			4.7		
	UR	73.0			21.9			3.4		
	UR	72.5	72.7	1.2	23.2	23.9	1.7	3.9	4.3	0.7
43	PH	71.1			23.4			5.2		
	UR	74.9	73.0	1.9	21.2	22.3	1.1	3.4	4.3	0.9
51	PH	71.8			21.9			4.4		
	PH	66.8			22.6			3.8		
	UR	73.2			18.8			3.6		
	UR	73.5	71.3	2.7	23.2	21.6	1.7	3.9	3.9	0.3
59	PH	70.8			22.6			5.2		
	PH	71.0			24.4			3.5		
	UR	77.4			18.3			3.3		
	UR	69.0	72.1	3.2	25.5	22.7	2.7	4.5	4.1	0.8
77	PH	71.5			21.0			5.8		
	PH	74.1			21.1			4.2		
	UR	71.5			21.4			3.8		
	UR	74.6	72.9	1.4	21.1	21.2	0.2	4.1	4.5	0.8
92	PH	73.1			20.0			5.5		
	PH	73.8			19.8			4.9		
	UR	74.0			20.6			3.7		
	UR	75.8	74.2	1.0	19.5	20.0	0.4	3.8	4.5	0.8

¹ Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Tables 4-5, pp. 43-44 of the study report.

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

[¹⁴C]Residue water phase:soil ratios.

Day ¹	Soil					[¹⁴ C]Residue Water Phase:Soil Ratios.							
	Ext.	Nonext.	Total in Soil			Water	Soil	Ratio	Ratio	W:S Ratio		S:W Ratio	
	% AR	% AR	% AR	Mean	s.d.	% AR	% AR	W:S	S:W	Mean	s.d.	Mean	s.d.
[Phenyl-U- ¹⁴ C]-label													
0	99.5	0.5	100.0										
	99.5	0.5	100.0	100.0	0.0								
14	93.8	5.8	99.6										
	90.5	6.8	97.3	98.5	1.2								
17	90.1	6.3	96.4										
	88.7	7.5	96.2	96.3	0.1								
23	26.8	4.8	31.6			63.9	31.6	2	0				
28	25.0	5.0	30.0			65.2	30.0	2	0				
	24.5	4.4	28.9	29.5	0.6	63.7	28.9	2	0	2	0	0	0
35	24.0	5.3	29.3			70.9	29.3	2	0				
	26.6	4.7	31.3	30.3	1.0	74.2	31.3	2	0	2	0	0	0
43	23.4	5.2	28.6			71.1	28.6	2	0				
51	21.9	4.4	26.3			71.8	26.3	3	0				
	22.6	3.8	26.4	26.4	0.1	66.8	26.4	3	0	3	0	0	0
59	22.6	5.2	27.8			70.8	27.8	3	0				
	24.4	3.5	27.9	27.9	0.0	71.0	27.9	3	0	3	0	0	0
77	21.0	5.8	26.8			71.5	26.8	3	0				
	21.1	4.2	25.3	26.1	0.7	74.1	25.3	3	0	3	0	0	0
92	20.0	5.5	25.5			73.1	25.5	3	0				
	19.8	4.9	24.7	25.1	0.4	73.8	24.7	3	0	3	0	0	0
[Uracil-4- ¹⁴ C]-label													
0	100.4	0.3	100.7										
	99.7	0.3	100.0	100.4	0.3								
14	91.8	4.4	96.2										
	93.6	5.4	99.0	97.6	1.4								
17	94.7	4.8	99.5										
	91.4	5.7	97.1	98.3	1.2								
23	25.1	3.5	28.6			69.7	28.6	2	0				
28	19.4	3.5	22.9			74.6	22.9	3	0				
	23.0	3.5	26.5	24.7	1.8	72.2	26.5	3	0	3	0	0	0
35	21.9	3.4	25.3			73.0	25.3	3	0				
	23.2	3.9	27.1	26.2	0.9	72.5	27.1	3	0	3	0	0	0
43	21.2	3.4	24.6			74.9	24.6	3	0				
51	18.8	3.6	22.4			73.2	22.4	3	0				
	23.2	3.9	27.1	24.8	2.4	73.5	27.1	3	0	3	0	0	0
59	18.3	3.3	21.6			77.4	21.6	4	0				
	25.5	4.5	30.0	25.8	4.2	69.0	30.0	2	0	3	1	0	0
77	21.4	3.8	25.2			71.5	25.2	3	0				
	21.1	4.1	25.2	25.2	0.0	74.6	25.2	3	0	3	0	0	0
92	20.6	3.7	24.3			74.0	24.3	3	0				
	19.5	3.8	23.3	23.8	0.5	75.8	23.3	3	0	3	0	0	0

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Tables 4-5, pp. 43-44 of the study report.

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

[^{14}C]Residue water phase:soil ratios for labels combined.

Day ¹	Label	Water	Soil	Ratio	Ratio	W:S Ratio		S:W Ratio	
		% AR	% AR	W:S	S:W	Mean	s.d.	Mean	s.d.
23	PH	63.9	31.6	2	0				
	UR	69.7	28.6	2	0	2	0	0	0
28	PH	65.2	30.0	2	0				
	PH	63.7	28.9	2	0				
	UR	74.6	22.9	3	0				
	UR	72.2	26.5	3	0	3	0	0	0
35	PH	70.9	29.3	2	0				
	PH	74.2	31.3	2	0				
	UR	73.0	25.3	3	0				
	UR	72.5	27.1	3	0	3	0	0	0
43	PH	71.1	28.6	2	0				
	UR	74.9	24.6	3	0	3	0	0	0
51	PH	71.8	26.3	3	0				
	PH	66.8	26.4	3	0				
	UR	73.2	22.4	3	0				
	UR	73.5	27.1	3	0	3	0	0	0
59	PH	70.8	27.8	3	0				
	PH	71.0	27.9	3	0				
	UR	77.4	21.6	4	0				
	UR	69.0	30.0	2	0	3	0	0	0
77	PH	71.5	26.8	3	0				
	PH	74.1	25.3	3	0				
	UR	71.5	25.2	3	0				
	UR	74.6	25.2	3	0	3	0	0	0
92	PH	73.1	25.5	3	0				
	PH	73.8	24.7	3	0				
	UR	74.0	24.3	3	0				
	UR	75.8	23.3	3	0	3	0	0	0

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results imported from **Ratios** worksheet.

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Confirmation/determination of means/std.dev. for saflufenacil and its transformation products.

[Phenyl-U- ^{14}C]-label.

Day ¹	Saflufenacil									M800H08								
	Water			Soil			Total system			Water			Soil			Total system		
	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0				93.8			93.8											
				104.4	99.1	5.3	104.4	99.1	5.3									
14				47.5			47.5						15.8			15.8		
				45.2	46.4	1.1	45.2	46.4	1.1				18.3	17.1	1.3	18.3	17.1	1.3
17				36.8			36.8						17.5			17.5		
				45.2	41.0	4.2	45.2	41.0	4.2				20.2	18.9	1.3	20.2	18.9	1.3
23	21.5			10.1			31.6			10.1			4.5			14.6		
28	19.4			8.4			27.8			15.7			7.5			23.2		
	17.3	18.4	1.0	14.4	11.4	3.0	31.7	29.8	2.0	15.3	15.5	0.2	3.8	5.7	1.9	19.1	21.2	2.1
35	19.4			7.3			26.7			18.7			6.4			25.1		
	44.8	32.1	12.7	16.1	11.7	4.4	60.9	43.8	17.1	10.3	14.5	4.2	3.8	5.1	1.3	14.1	19.6	5.5
43	49.5			14.3			63.8			8.5			2.6			11.1		
51	22.4			6.2			28.6			12.2			3.4			15.6		
	47.5	35.0	12.6	14.6	10.4	4.2	62.1	45.4	16.8	8.2	10.2	2.0	2.8	3.1	0.3	11.0	13.3	2.3
59	19.4			6.5			25.9			14.2			3.8			18.0		
	54.2	36.8	17.4	17.8	12.2	5.7	72.0	49.0	23.1	8.1	11.2	3.1	2.5	3.2	0.7	10.6	14.3	3.7
77	21.4			6.7			28.1			14.4			4.5			18.9		
	49.9	35.7	14.3	12.1	9.4	2.7	62.0	45.1	17.0	8.3	11.4	3.1	2.6	3.6	1.0	10.9	14.9	4.0
92	20.8			5.3			26.1			14.1			3.4			17.5		
	30.5	25.7	4.9	7.3	6.3	1.0	37.8	32.0	5.8	20.0	17.1	2.9	5.4	4.4	1.0	25.4	21.5	4.0

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 6, pp. 45-47 of the study report.

Bolded results are those samples (Replicate 2 samples) study authors believed degradation was affected by loss of soil moisture during aerobic incubation.

Blank cell = not applicable (NA) or not detected (ND).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

Confirmation/determination of means/std.dev. for saflufenacil and its transformation products.

[Phenyl-U-¹⁴C]-label (continued).

Day ¹	M800H01									M800H02								
	Water			Soil			Total system			Water			Soil			Total system		
	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0																		
14				14.1			14.1						18.0			18.0		
				10.3	12.2	1.9	10.3	12.2	1.9				7.2	12.6	5.4	7.2	12.6	5.4
17				11.6			11.6						14.6			14.6		
				7.5	9.6	2.1	7.5	9.6	2.1				5.4	10.0	4.6	5.4	10.0	4.6
23	9.4			3.2			12.6			12.8			3.6			16.4		
28	8.7			2.3			11.0			11.8			4.1			15.9		
	7.3	8.0	0.7	1.9	2.1	0.2	9.2	10.1	0.9	12.6	12.2	0.4	1.8	3.0	1.2	14.4	15.2	0.8
35	9.3			2.4			11.7			13.7			4.0			17.7		
	7.6	8.5	0.9	1.9	2.2	0.3	9.5	10.6	1.1	4.9	9.3	4.4	1.3	2.7	1.4	6.2	12.0	5.8
43	3.9			11.0			14.9			3.2			0.8			4.0		
51	11.0			2.5			13.5			16.3			4.0			20.3		
	4.1	7.6	3.5	1.1	1.8	0.7	5.2	9.4	4.2	1.8	9.1	7.3	0.6	2.3	1.7	2.4	11.4	9.0
59	9.8			2.0			11.8			15.2			4.2			19.4		
	3.0	6.4	3.4	1.1	1.6	0.5	4.1	8.0	3.9	1.2	8.2	7.0	0.7	2.5	1.8	1.9	10.7	8.8
77	7.5			2.0			9.5			17.2			4.5			21.7		
	5.5	6.5	1.0	1.1	1.6	0.5	6.6	8.1	1.5	3.2	10.2	7.0	0.8	2.7	1.9	4.0	12.9	8.9
92	8.2			1.8			10.0			19.8			4.2			24.0		
	5.8	7.0	1.2	1.3	1.6	0.3	7.1	8.6	1.5	8.3	14.1	5.8	1.3	2.8	1.5	9.6	16.8	7.2

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 6, pp. 45-47 of the study report.

Bolded results are those samples (Replicate 2 samples) study authors believed degradation was affected by loss of soil moisture during aerobic incubation.

Blank cell = not applicable (NA) or not detected (ND).

Shaded block indicates result does not agree (>0.1%) with that reported by the study authors (Reviewer's Comment No. 1).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)
 PC: 118203
 MRID: 47611201
 Guideline: 835.4200

**Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.
 Confirmation/determination of means/std.dev. for saflufenacil and its transformation products.
 [Phenyl-U-¹⁴C]-label (continued).**

Day ¹	M800H07						M800H15 ketohydrate						M800H22		
	Water			Soil			Water			Soil			Total system		
	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0															
14				1.8	2.2	0.2				1.3	1.8	0.5	1.3		
17				2.2	2.0	0.2				2.3	1.8	0.5	2.3		
				1.5	3.7	1.1				1.1	1.1	0.0	1.1		
23	2.6			3.7	2.6	1.1									
				0.9	3.5		0.8						0.8		
28	2.5			1.2	3.7		1.1			0.4	0.5	0.1	1.5		
	1.8	2.2	0.4	0.8	2.6	0.5		1.1	0.0	0.5	1.0	0.5	0.5		
35	2.5			1.0	3.5										
		2.5	0.0	1.1	2.3	1.2				0.3	0.3	0.0	0.3		
43	2.2			1.1	3.0					0.4			0.4		
51	2.1			0.8	3.0										
	1.7	1.9	0.2	1.3	3.0	0.0									
59	2.8			1.1	3.9										
	1.2	2.0	0.8	0.7	1.9	1.0				0.3	0.3	0.0	0.3		
77	3.3			1.1	4.4		0.9								
	1.8	2.6	0.8	0.6	2.4	1.0		0.9	0.0	0.2	0.2	0.0	0.9		
92	1.3			0.2	1.5					0.2	0.2	0.0	0.2		
	2.4	1.9	0.6	0.9	3.3	0.9				0.4	0.3	0.1	0.4		
					2.4	0.9									

¹ Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 6, pp. 45-47 of the study report.

Bolded results are those samples (Replicate 2 samples) study authors believed degradation was affected by loss of soil moisture during aerobic incubation.

Blank cell = not applicable (NA) or not detected (ND).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Unidentified [^{14}C]residues.

[Phenyl- $\text{U-}^{14}\text{C}$]-label.

Day ¹	Water layer							Soil							Total system						
	UNK 25.8	UNK 26.3	UNK 26.6	Other	Total			UNK 25.8	UNK 26.3	UNK 26.6	Other	Total			UNK 25.8	UNK 26.3	UNK 26.6	Other	Total		
	% AR	% AR	% AR	% AR	% AR	mean	s.d.	% AR	% AR	% AR	% AR	% AR	mean	s.d.	% AR	% AR	% AR	% AR	% AR	mean	s.d.
0											2.1	2.1			0.0	0.0	0.0	2.1	2.1		
											2.7	2.7	2.4	0.3	0.0	0.0	0.0	2.7	2.7	2.4	0.3
14									2.1	3.9	1.5	7.5			0.0	2.1	3.9	1.5	7.5		
									1.5	4.0		5.5	6.5	1.0	0.0	1.5	4.0	0.0	5.5	6.5	1.0
17								1.2	1.4		2.4	5.0			1.2	1.4	0.0	2.4	5.0		
								1.0				1.0	3.0	2.0	1.0	0.0	0.0	0.0	1.0	3.0	2.0
23	1.1	3.9			5.0			0.4	1.0		0.3	1.7			1.5	4.9	0.0	0.3	6.7		
28	1.1	2.8			3.9				0.8		0.6	1.4			1.1	3.6	0.0	0.6	5.3		
	1.1	2.7		3.7	7.5	5.7	1.8		0.9			0.9	1.2	0.3	1.1	3.6	0.0	3.7	8.4	6.9	1.6
35	1.0	3.6		0.7	5.3			0.8	1.0		1.1	2.9			1.8	4.6	0.0	1.8	8.2		
		2.7		1.5	4.2	4.8	0.6		0.6	0.2	0.4	1.2	2.1	0.9	0.0	3.3	0.2	1.9	5.4	6.8	1.4
43		1.8			1.8				0.4		0.3	0.7			0.0	2.2	0.0	0.3	2.5		
51		2.5		0.6	3.1				0.2	1.0	1.4	2.6			0.0	2.7	1.0	2.0	5.7		
		1.4			1.4	2.3	0.9			1.4		1.4	2.0	0.6	0.0	1.4	1.4	0.0	2.8	4.3	1.5
59		1.4	3.5	2.5	7.4				0.4	1.0	0.7	2.1			0.0	1.8	4.5	3.2	9.5		
			1.2		1.2	4.3	3.1			1.2		1.2	1.7	0.4	0.0	0.0	2.4	0.0	2.4	6.0	3.6
77		1.7	3.7		5.4			0.3	1.0		0.8	2.1			0.3	2.7	3.7	0.8	7.5		
			2.3		2.3	3.9	1.6	0.3	0.7	0.7	0.9	2.6	2.4	0.3	0.3	0.7	3.0	0.9	4.9	6.2	1.3
92	1.5	3.1			4.6			0.4		0.9	2.2	3.5			1.9	3.1	0.9	2.2	8.1		
		3.3			3.3	4.0	0.7		1.0		1.1	2.1	2.8	0.7	0.0	4.3	0.0	1.1	5.4	6.8	1.4

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 6, pp. 45-47 of the study report.

Bolded results are those samples (Replicate 2 samples) study authors believed degradation was affected by loss of soil moisture during aerobic incubation.

Blank cell = not applicable (NA) or not detected (ND).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

[¹⁴C]Residues unaccounted for following HPLC.

[Phenyl-U-¹⁴C]-label.

Day ¹	Water layer										
	Initial % AR	Parent % AR	M800H-					Unided % AR	Unaccounted for Residues		
			08 % AR	01 % AR	02 % AR	07 % AR	15 % AR		% AR	mean	s.d.
0											
14											
17											
23	63.9	21.5	10.1	9.4	12.8	2.6	0.8	5.0	1.7		
28	65.2	19.4	15.7	8.7	11.8	2.5	1.1	3.9	2.1		
	63.7	17.3	15.3	7.3	12.6	1.8		7.5	1.9	2.0	0.1
35	70.9	19.4	18.7	9.3	13.7	2.5		5.3	2.0		
	74.2	44.8	10.3	7.6	4.9			4.2	2.4	2.2	0.2
43	71.1	49.5	8.5	3.9	3.2	2.2		1.8	2.0		
51	71.8	22.4	12.2	11.0	16.3	2.1		3.1	4.7		
	66.8	47.5	8.2	4.1	1.8	1.7		1.4	2.1	3.4	1.3
59	70.8	19.4	14.2	9.8	15.2	2.8		7.4	2.0		
	71.0	54.2	8.1	3.0	1.2	1.2		1.2	2.1	2.1	0.1
77	71.5	21.4	14.4	7.5	17.2	3.3	0.9	5.4	1.4		
	74.1	49.9	8.3	5.5	3.2	1.8		2.3	3.1	2.3	0.8
92	73.1	20.8	14.1	8.2	19.8	1.3		4.6	4.3		
	73.8	30.5	20.0	5.8	8.3	2.4		3.3	3.5	3.9	0.4

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 4, p. 43; Table 6, pp. 45-47 of the study report.

Unided results imported from **Unided** PH worksheet.

Bolded results are those samples (Replicate 2 samples) study authors believed degradation was affected by loss of soil moisture during aerobic incubation.

Blank cell = not applicable (NA) or not detected (ND).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

[¹⁴C]Residues unaccounted for following HPLC.

[Phenyl-U-¹⁴C]-label (continued).

Day ¹	Soil											
	Initial	Parent	M800H-						Unided	Unaccounted for Residues		
			08	01	02	07	15	22		% AR	mean	s.d.
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR		
0	99.5	93.8							2.1	3.6		
	99.5	104.4							2.7	-7.6	-2.0	5.6
14	93.8	47.5	15.8	14.1	18.0	1.8	1.3		7.5	-12.2		
	90.5	45.2	18.3	10.3	7.2	2.2	2.3		5.5	-0.5	-6.4	5.9
17	90.1	36.8	17.5	11.6	14.6	1.5	1.1		5.0	2.0		
	88.7	45.2	20.2	7.5	5.4	3.7			1.0	5.7	3.9	1.9
23	26.8	10.1	4.5	3.2	3.6	0.9			1.7	2.8		
28	25.0	8.4	7.5	2.3	4.1	1.2	0.4		1.4	-0.3		
	24.5	14.4	3.8	1.9	1.8	0.8	0.5		0.9	0.4	0.1	0.3
35	24.0	7.3	6.4	2.4	4.0	1.0			2.9	0.0		
	26.6	16.1	3.8	1.9	1.3	1.1	0.3		1.2	0.9	0.5	0.5
43	23.4	14.3	2.6	11.0	0.8	0.8	0.4		0.7	-7.2		
51	21.9	6.2	3.4	2.5	4.0	0.9			2.6	2.3		
	22.6	14.6	2.8	1.1	0.6	1.3			1.4	0.8	1.6	0.7
59	22.6	6.5	3.8	2.0	4.2	1.1			2.1	2.9		
	24.4	17.8	2.5	1.1	0.7	0.7	0.3		1.2	0.1	1.5	1.4
77	21.0	6.7	4.5	2.0	4.5	1.1		0.3	2.1	-0.2		
	21.1	12.1	2.6	1.1	0.8	0.6	0.2		2.6	1.1	0.5	0.7
92	20.0	5.3	3.4	1.8	4.2	0.2	0.2	0.2	3.5	1.2		
	19.8	7.3	5.4	1.3	1.3	0.9	0.4	0.4	2.1	0.7	0.9	0.2

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 4, p. 43; Table 6, pp. 45-47 of the study report.

Unided results imported from Unided PH worksheet.

Bolded results are those samples (Replicate 2 samples) study authors believed degradation was affected by loss of soil moisture during aerobic incubation.

Blank cell = not applicable (NA) or not detected (ND).

Study authors reported HPLC analyses and peak calculations used soil concentrates which differed from initial extract within 90-117% (pp. 31-32).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

Confirmation/determination of means/std.dev. for saflufenacil and its transformation products.

[Uracil-4-¹⁴C]-label.

Day ¹	Saflufenacil									M800H08								
	Water			Soil			Total system			Water			Soil			Total system		
	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0				111	114	3	111	114	3									
14				53.8	49.8	4.1	53.8	49.8	4.1				13.1	14.1	0.9	13.1		
17				45.7	49.8	4.1	45.7	49.8	4.1				15.0	14.1	0.9	15.0	14.1	0.9
17				48.2	44.3	4.0	48.2	44.3	4.0				11.8	14.6	2.8	11.8		
23	31.1			40.3	44.3	4.0	40.3	44.3	4.0				17.4	14.6	2.8	17.4	14.6	2.8
28	29.1			12.3			43.4			10.1			4.4			14.5		
28	28.5	28.8	0.3	7.9			37.0			17.4			5.2			22.6		
35	30.9			11.4	9.7	1.8	39.9	38.5	1.4	8.5	13.0	4.5	4.2	4.7	0.5	12.7	17.7	5.0
35	27.9	29.4	1.5	11.1	10.7	0.4	42.0	40.1	1.9	15.8			5.8			21.6		
43	28.7			10.3			38.2	40.1	1.9	13.7	14.8	1.1	5.2	5.5	0.3	18.9	20.3	1.4
51	27.8			10.0			38.7			13.7			4.7			18.4		
51	27.7	27.8	0.1	7.0			34.8			14.0			3.6			17.6		
59	27.3			9.5	8.3	1.3	37.2	36.0	1.2	14.7	14.4	0.4	5.6	4.6	1.0	20.3	19.0	1.4
59	26.6	27.0	0.3	6.2			33.5			18.0			3.3			21.3		
77	25.8			11.3	8.8	2.6	37.9	35.7	2.2	15.5	16.8	1.3	5.6	4.5	1.2	21.1	21.2	0.1
77	25.6	25.7	0.1	8.7			34.5			15.3			5.7			21.0		
92	25.8			7.2	8.0	0.8	32.8	33.7	0.8	18.5	16.9	1.6	5.4	5.6	0.1	23.9	22.5	1.5
92	27.8	26.8	1.0	8.5			34.3			13.5			4.4			17.9		
				8.0	8.3	0.3	35.8	35.1	0.8	18.5	16.0	2.5	5.0	4.7	0.3	23.5	20.7	2.8

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Confirmation/determination of means/std.dev. for saflufenacil and its transformation products.

[Uracil-4- ^{14}C]-label (continued).

Day ¹	M800H01									M800H02								
	Water			Soil			Total system			Water			Soil			Total system		
	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0																		
14				9.0			9.0						8.4			8.4		
				12.3	10.7	1.7	12.3	10.7	1.7				12.6	10.5	2.1	12.6	10.5	2.1
17				11.3			11.3						14.4			14.4		
				9.9	10.6	0.7	9.9	10.6	0.7				12.0	13.2	1.2	12.0	13.2	1.2
23	7.4			2.3			9.7			13.0			2.8			15.8		
28	6.5			1.4			7.9			15.0			3.0			18.0		
	9.4	8.0	1.5	2.2	1.8	0.4	11.6	9.8	1.9	16.1	15.6	0.6	4.5	3.8	0.8	20.6	19.3	1.3
35	7.5			2.2			9.7			9.8			2.8			12.6		
	8.4	8.0	0.5	2.6	2.4	0.2	11.0	10.4	0.7	15.3	12.6	2.8	4.6	3.7	0.9	19.9	16.3	3.7
43	9.4			2.3			11.7			10.4			2.9			13.3		
51	6.9			1.6			8.5			18.5			4.0			22.5		
	8.7	7.8	0.9	2.5	2.1	0.5	11.2	9.9	1.4	12.1	15.3	3.2	3.9	4.0	0.1	16.0	19.3	3.3
59	8.7			1.4			10.1			18.0			3.4			21.4		
	8.2	8.5	0.3	2.3	1.9	0.5	10.5	10.3	0.2	10.6	14.3	3.7	3.6	3.5	0.1	14.2	17.8	3.6
77	7.9			2.2			10.1			14.1			4.1			18.2		
	9.2	8.6	0.6	2.1	2.2	0.0	11.3	10.7	0.6	13.3	13.7	0.4	3.2	3.7	0.5	16.5	17.4	0.8
92	7.9			2.0			9.9			17.0			4.3			21.3		
	10.3	9.1	1.2	1.9	2.0	0.0	12.2	11.1	1.2	13.9	15.5	1.6	3.1	3.7	0.6	17.0	19.2	2.2

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 7, pp. 48-50 of the study report.

Blank cell = not applicable (NA) or not detected (ND).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Salfufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]salfufenacil in Wisconsin loamy sand soil.

Confirmation/determination of means/std.dev. for salfufenacil and its transformation products.

[Uracyl-4-¹⁴C]-label (continued).

Day ¹	M800H15 ketohydrate						M800H22					
	Water			Soil			Total system			Water		
	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0												
14				1.7	1.7	0.0						
17												
23	1.2											
28	0.8						1.2					
	0.9	0.9	0.0				0.8					
							0.9	0.9	0.0			
35	1.6	1.6	0.0	0.3	0.3	0.0	1.9					
								1.9	0.0			
43				0.3			0.3					
51				0.9			0.9					
				1.2	1.1	0.2	1.2	1.1	0.2			
59				0.2			0.2					
				0.5	0.4	0.2	0.5	0.4	0.2			
77				0.2	0.2	0.0	0.2	0.2	0.0	1.6	1.6	0.0
92										0.2	0.2	0.0
										0.2	0.2	0.0

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 7, pp. 48-50 of the study report.

Blank cell = not applicable (NA) or not detected (ND).

Shaded block indicates result does not agree (>0.1%) with that reported by the study authors (Reviewer's Comment No. 1).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

Confirmation/determination of means/std.dev. for saflufenacil and its transformation products.

[Uracil-4- ^{14}C]-label.

Day ¹	Trifluoroacetic acid								
	Water			Soil			Total system		
	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0									
14				2.7			2.7		
				2.7	2.7	0.0	2.7	2.7	0.0
17				4.8			4.8		
				6.9	5.9	1.1	6.9	5.9	1.1
23	2.6						2.6		
28	1.9			0.5			2.4		
	3.2	2.6	0.7		0.5	0.0	3.2	2.8	0.4
35							0.0		
	3.1	3.1	0.0				3.1	1.6	1.6
43	2.4						2.4		
51	2.3						2.3		
	2.7	2.5	0.2	0.8	0.8	0.0	3.5	2.9	0.6
59	1.5			0.8			2.3		
	1.7	1.6	0.1	1.0	0.9	0.1	2.7	2.5	0.2
77	3.4			0.6			4.0		
	2.7	3.1	0.4	0.7	0.7	0.1	3.4	3.7	0.3
92	1.6			0.9			2.5		
	2.8	2.2	0.6	0.9	0.9	0.0	3.7	3.1	0.6

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 7, pp. 48-50 of the study report.

Blank cell = not applicable (NA) or not detected (ND).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

Unidentified [¹⁴C]residues.

[Uracil-4-¹⁴C]-label.

Day ¹	Water layer							Soil							Total system						
	UNK 25.8	UNK 26.3	UNK 26.6	Other	Total			UNK 25.8	UNK 26.3	UNK 26.6	Other	Total			UNK 25.8	UNK 26.3	UNK 26.6	Other	Total		
	% AR	% AR	% AR	% AR	% AR	mean	s.d.	% AR	% AR	% AR	% AR	% AR	mean	s.d.	% AR	% AR	% AR	% AR	% AR	mean	s.d.
0															0.0	0.0	0.0	0.0	0.0	0.0	0.0
14										3.1		3.1	3.7	0.6	0.0	0.0	3.1	0.0	3.1	3.7	0.6
17										4.3		4.3			0.0	0.0	4.3	0.0	4.3		
										3.7		3.7			0.0	0.0	3.7	0.0	3.7		
										3.8		3.8	3.8	0.0	0.0	0.0	3.8	0.0	3.8	3.8	0.0
23	1.5	2.7			4.2				0.8			0.8			1.5	3.5	0.0	0.0	5.0		
28	1.4	2.5			3.9				0.8			0.8			1.4	3.3	0.0	0.0	4.7		
	1.1	3.1		1.3	5.5	4.7	0.8	0.3	0.9		0.3	1.5	1.2	0.4	1.4	4.0	0.0	1.6	7.0	5.9	1.2
35	1.4	2.6		3.3	7.3				0.8			0.8			1.4	3.4	0.0	3.3	8.1		
	1.1	3.1			4.2	5.8	1.6	0.5	0.8			1.3	1.1	0.3	1.6	3.9	0.0	0.0	5.5	6.8	1.3
43	0.9	2.4		6.8	10.1			0.4	1.0		0.7	2.1			1.3	3.4	0.0	7.5	12.2		
51	0.9	2.7			3.6				0.4		1.3	1.7			0.9	3.1	0.0	1.3	5.3		
	1.7	4.5		1.6	7.8	5.7	2.1				2.2	2.2	2.0	0.3	1.7	4.5	0.0	3.8	10.0	7.7	2.4
59		0.9	2.3	0.8	4.0					0.5	1.3	1.8			0.0	0.9	2.8	2.1	5.8		
		1.6	2.6	2.4	6.6	5.3	1.3			1.2	0.7	1.9	1.9	0.0	0.0	1.6	3.8	3.1	8.5	7.2	1.4
77		1.3	2.1		3.4			0.3	0.7			1.0			0.3	2.0	2.1	0.0	4.4		
		1.1	0.7		1.8	2.6	0.8	0.3	0.8		0.4	1.5	1.3	0.3	0.3	1.9	0.7	0.4	3.3	3.9	0.6
92	2.2	2.6		2.7	7.5			0.3	0.7			1.0			2.5	3.3	0.0	2.7	8.5		
	1.3	2.6			3.9	5.7	1.8		0.5		0.1	0.6	0.8	0.2	1.3	3.1	0.0	0.1	4.5	6.5	2.0

¹ Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 7, pp. 48-50 of the study report.

Blank cell = not applicable (NA) or not detected (ND).

Shaded block indicates result does not agree (>0.1%) with that reported by the study authors (Reviewer's Comment No. 1).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [¹⁴C]saflufenacil in Wisconsin loamy sand soil.

[¹⁴C]Residues unaccounted for following HPLC.

[Uracil-4-¹⁴C]-label.

Day ¹	Water layer											
	Initial	Parent	M800H-						Unided	Unaccounted for		
			08	01	02	15	22	TFA		Residues		
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	mean	s.d.
0												
14												
17												
23	69.7	31.1	10.1	7.4	13.0	1.2		2.6	4.2	0.1		
28	74.6	29.1	17.4	6.5	15.0	0.8		1.9	3.9	0.0		
	72.2	28.5	8.5	9.4	16.1	0.9		3.2	5.5	0.1	0.0	0.1
35	73.0	30.9	15.8	7.5	9.8	1.6			7.3	0.1		
	72.5	27.9	13.7	8.4	15.3			3.1	4.2	-0.1	0.0	0.1
43	74.9	28.7	13.7	9.4	10.4			2.4	10.1	0.2		
51	73.2	27.8	14.0	6.9	18.5			2.3	3.6	0.1		
	73.5	27.7	14.7	8.7	12.1			2.7	7.8	-0.2	0.0	0.2
59	77.4	27.3	18.0	8.7	18.0			1.5	4.0	-0.1		
	69.0	26.6	15.5	8.2	10.6			1.7	6.6	-0.2	-0.1	0.1
77	71.5	25.8	15.3	7.9	14.1		1.6	3.4	3.4	0.0		
	74.6	25.6	18.5	9.2	13.3		1.6	2.7	1.8	1.9	0.9	0.9
92	74.0	25.8	13.5	7.9	17.0			1.6	7.5	0.7		
	75.8	27.8	18.5	10.3	13.9			2.8	3.9	-1.4	-0.3	1.1

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 5, p. 44; Table 7, pp. 48-50 of the study report.

Unided results imported from **Unided UR** worksheet.

Blank cell = not applicable (NA) or not detected (ND).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Saflufenacil (BAS 800 H)

PC: 118203

MRID: 47611201

Guideline: 835.4200

Anaerobic metabolism of [^{14}C]saflufenacil in Wisconsin loamy sand soil.

[^{14}C]Residues unaccounted for following HPLC.

[Uracil-4- ^{14}C]-label (continued).

Day ¹	Soil											
	Initial	Parent	M800H-						Unided	Unaccounted for		
			08	01	02	15	22	TFA		Residues		
	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	mean	s.d.
0	100.4	111							0.0	-10.6		
	99.7	117							0.0	-17.3	-14.0	3.4
14	91.8	53.8	13.1	9.0	8.4			2.7	3.1	1.7		
	93.6	45.7	15.0	12.3	12.6	1.7		2.7	4.3	-0.7	0.5	1.2
17	94.7	48.2	11.8	11.3	14.4			4.8	3.7	0.5		
	91.4	40.3	17.4	9.9	12.0			6.9	3.8	1.1	0.8	0.3
23	25.1	12.3	4.4	2.3	2.8				0.8	2.5		
28	19.4	7.9	5.2	1.4	3.0			0.5	0.8	0.6		
	23.0	11.4	4.2	2.2	4.5				1.5	-0.8	-0.1	0.7
35	21.9	11.1	5.8	2.2	2.8	0.3			0.8	-1.1		
	23.2	10.3	5.2	2.6	4.6				1.3	-0.8	-1.0	0.2
43	21.2	10.0	4.7	2.3	2.9	0.3			2.1	-1.1		
51	18.8	7.0	3.6	1.6	4.0	0.9			1.7	0.0		
	23.2	9.5	5.6	2.5	3.9	1.2		0.8	2.2	-2.5	-1.3	1.3
59	18.3	6.2	3.3	1.4	3.4	0.2		0.8	1.8	1.2		
	25.5	11.3	5.6	2.3	3.6	0.5		1.0	1.9	-0.7	0.3	1.0
77	21.4	8.7	5.7	2.2	4.1			0.6	1.0	-0.9		
	21.1	7.2	5.4	2.1	3.2	0.2		0.7	1.5	0.8	0.0	0.9
92	20.6	8.5	4.4	2.0	4.3		0.2	0.9	1.0	-0.7		
	19.5	8.0	5.0	1.9	3.1		0.2	0.9	0.6	-0.2	-0.5	0.2

1 Days posttreatment; treated soil flooded after 17 days of aerobic incubation.

Results from Table 5, p. 44; Table 7, pp. 48-50 of the study report.

Unided results imported from Unided UR worksheet.

Blank cell = not applicable (NA) or not detected (ND).

Study authors reported HPLC analyses and peak calculations used soil concentrates which differed from initial extract within 90-117% (pp. 31-32).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Guideline: 835.4200

Anaerobic metabolism of 14 C isafufenacil in Wisconsin loamy sand soil.

Determination of means/std.dev. for saflufenacil and products with labels combined.

[illegible]

	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9	Day 10	Day 11	Day 12	Day 13	Day 14	Day 15	Day 16	Day 17	Day 18	Day 19	Day 20	Day 21	Day 22	Day 23	Day 24	Day 25	Day 26	Day 27	Day 28	Day 29	Day 30	Day 31	Day 32	Day 33	Day 34	Day 35	Day 36	Day 37	Day 38	Day 39	Day 40	Day 41	Day 42	Day 43	Day 44	Day 45	Day 46	Day 47	Day 48	Day 49	Day 50	Day 51	Day 52	Day 53	Day 54	Day 55	Day 56	Day 57	Day 58	Day 59	Day 60	Day 61	Day 62	Day 63	Day 64	Day 65	Day 66	Day 67	Day 68	Day 69	Day 70	Day 71	Day 72	Day 73	Day 74	Day 75	Day 76	Day 77	Day 78	Day 79	Day 80	Day 81	Day 82	Day 83	Day 84	Day 85	Day 86	Day 87	Day 88	Day 89	Day 90	Day 91	Day 92	Day 93	Day 94	Day 95	Day 96	Day 97	Day 98	Day 99	Day 100
1	Days posttreatment: treated soil flooded after 17 days of aerobic incubation.																																																																																																			

1 Days posttreatment, treated soil incubated after 17 days of aerobic incubation.
Results from Tables 6-7, pp. 45-50 of the study report: blank cell = not applicable (NA) or not detected (ND).

Results from Tables 6-7, pp. 43-50 of the study report, blank cell = not applicable (NA), not detected (ND).

Bolded results are those samples (Replicate 2 samples) study authors believed degradation was affected by loss of A1:A2. Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

**Attachment 3: Transformation Pathway Presented by Registrant
Illustration of Test System**

Figure 27. Metabolic pathway in aerobic followed by anaerobic metabolism of BAS 800 H

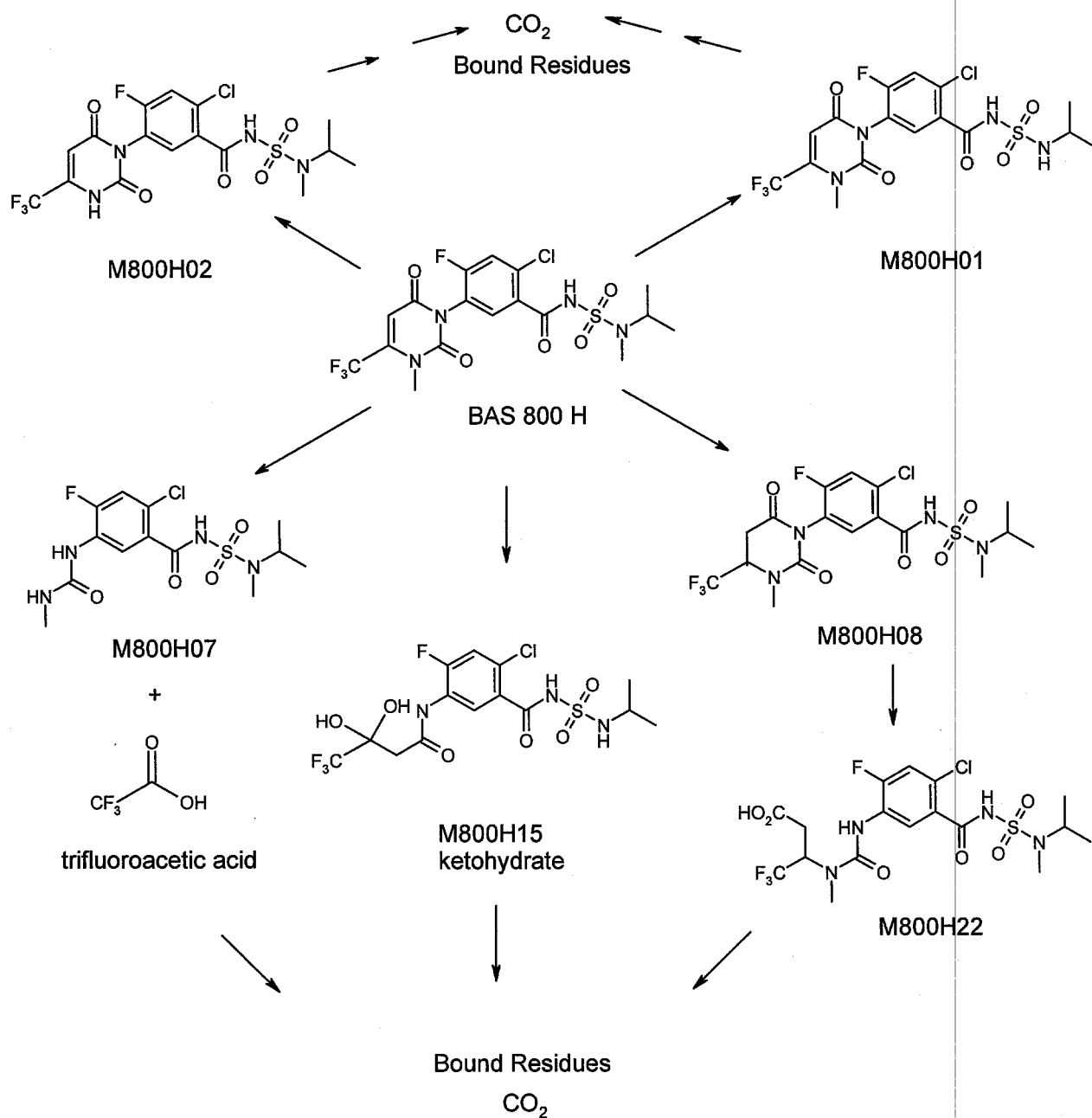
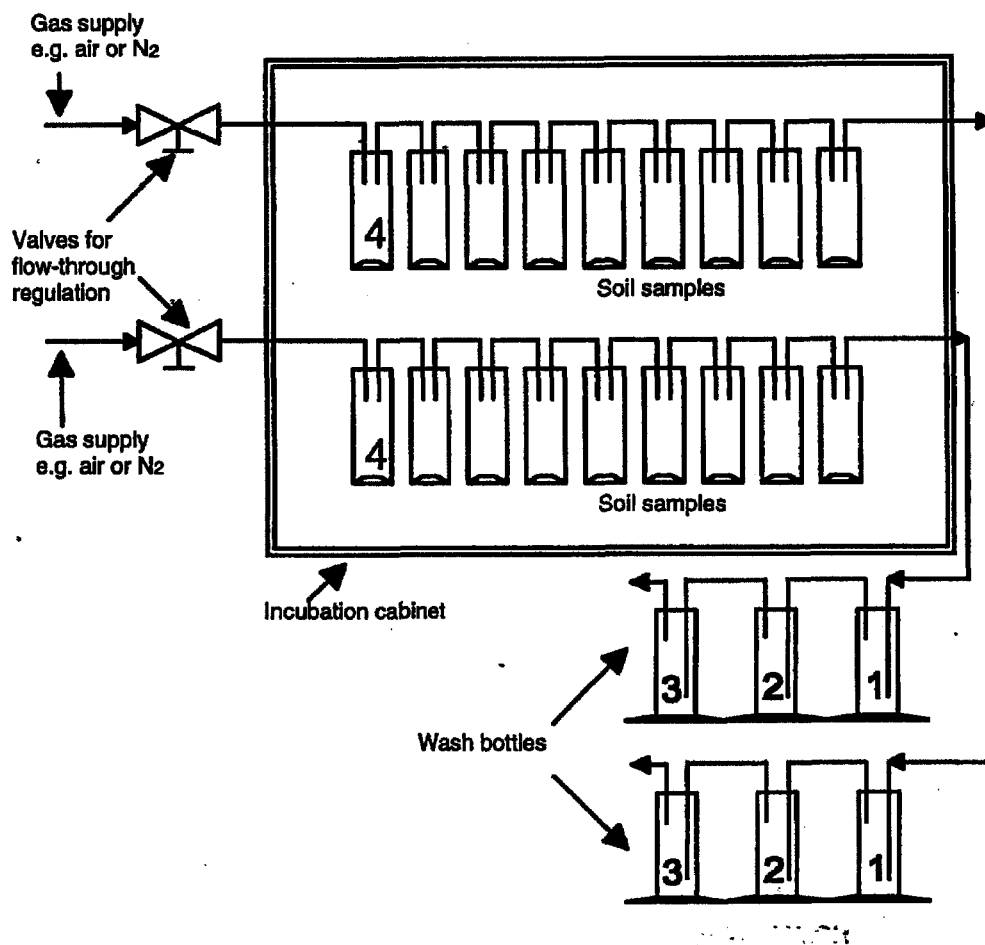


Figure 3. Diagram of sample set-up



This sketch provides a general view of the setup and does not necessarily reflect the exact setup in the study. Soil was in the containers for the aerobic phase and air was drawn through with a vacuum with air exiting through the wash bottles containing trapping solution. For the anaerobic phase soil and water were in each sample container and the nitrogen flow passed over and not into the water, exiting through the wash bottles containing trapping solution. Sample series were set up with the lowest container ID, e.g. UR01 and UR12, closest to the wash bottles.

Incubation in aerobic phase: 4 contained 0.5N NaOH
1 and 2 contained 0.5N NaOH
3 was not used

Incubation in anaerobic phase: 4 contained water
1 contained ethylene glycol
2 contained 0.5N NaOH
3 was not used